Applicants: Wayne A. Hendrickson , et al.
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Filing Date: June 29, 2000
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FIGURE 8A-1

```
HEADER      GROWTH FACTOR                                               1SCF
TITLE       HUMAN RECOMBINANT STEM CELL FACTOR
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: STEM CELL FACTOR;
COMPND      3 CHAIN: A, B, C, D;
COMPND      4 SYNONYM: SCF, SL, MGF, MAST CELL GROWTH FACTOR;
COMPND      5 ENGINEERED: YES;
COMPND      6 BIOLOGICAL_UNIT: DIMER
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      3 ORGANISM_COMMON: HUMAN;
SOURCE      4 EXPRESSION_SYSTEM: NULL
KEYWDS      HUMAN STEM CELL FACTOR, STEEL FACTOR, KIT LIGAND, MAST CELL
KEYWDS      2 GROWTH FACTOR
EXPDTA      X-RAY DIFFRACTION
AUTHOR      X.JIANG,O.GUREL,K.E.LANGLEY,W.A.HENDRICKSON
JRNL            AUTH   X.JIANG,O.GUREL,K.E.LANGLEY,W.A.HENDRICKSON
JRNL            TITL   CRYSTAL STRUCTURE OF RECOMBINANT HUMAN STEM CELL
JRNL            TITL 2 FACTOR
JRNL            REF    TO BE PUBLISHED
JRNL            REFN                                                    0353
REMARK   1
REMARK   2
REMARK   2 RESOLUTION. 2.2  ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3    PROGRAM       : X-PLOR 3.1
REMARK   3    AUTHORS       : BRUNGER
REMARK   3
REMARK   3 DATA USED IN REFINEMENT.
REMARK   3    RESOLUTION RANGE HIGH (ANGSTROMS) : 2.2
REMARK   3    RESOLUTION RANGE LOW  (ANGSTROMS) : 20.0
REMARK   3    DATA CUTOFF            (SIGMA(F)) : 2
REMARK   3    DATA CUTOFF HIGH        (ABS(F)) : 100000
REMARK   3    DATA CUTOFF LOW         (ABS(F)) : 0.1
REMARK   3    COMPLETENESS (WORKING+TEST)   (%) : 96.6
REMARK   3    NUMBER OF REFLECTIONS             : 49851
REMARK   3
REMARK   3 FIT TO DATA USED IN REFINEMENT.
REMARK   3    CROSS-VALIDATION METHOD         : THROUGHOUT
REMARK   3    FREE R VALUE TEST SET SELECTION : RANDOM
REMARK   3    R VALUE            (WORKING SET) : 0.199
REMARK   3    FREE R VALUE                     : 0.242
REMARK   3    FREE R VALUE TEST SET SIZE   (%) : 6.0
REMARK   3    FREE R VALUE TEST SET COUNT      : 3016
REMARK   3    ESTIMATED ERROR OF FREE R VALUE  : 0.0044
REMARK   3
REMARK   3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3    TOTAL NUMBER OF BINS USED        : 10
REMARK   3    BIN RESOLUTION RANGE HIGH    (A) : 2.0
REMARK   3    BIN RESOLUTION RANGE LOW     (A) : 2.28
REMARK   3    BIN COMPLETENESS (WORKING+TEST) (%) : 97.0
REMARK   3    REFLECTIONS IN BIN   (WORKING SET) : 4349
REMARK   3    BIN R VALUE          (WORKING SET) : 0.3159
REMARK   3    BIN FREE R VALUE                  : 0.3450
REMARK   3    BIN FREE R VALUE TEST SET SIZE  (%) : 6.4
REMARK   3    BIN FREE R VALUE TEST SET COUNT  : 302
REMARK   3    ESTIMATED ERROR OF BIN FREE R VALUE : 0.0198
REMARK   3
REMARK   3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
```

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FIGURE 8A-2

```
REMARK   3   PROTEIN ATOMS              : 3517
REMARK   3   NUCLEIC ACID ATOMS         : 0
REMARK   3   HETEROGEN ATOMS            : 19
REMARK   3   SOLVENT ATOMS              : 264
REMARK   3
REMARK   3   B VALUES.
REMARK   3    FROM WILSON PLOT          (A**2)  : 38.5
REMARK   3    MEAN B VALUE        (OVERALL, A**2) : 32.1
REMARK   3    OVERALL ANISOTROPIC B VALUE.
REMARK   3     B11 (A**2)  : NULL
REMARK   3     B22 (A**2)  : NULL
REMARK   3     B33 (A**2)  : NULL
REMARK   3     B12 (A**2)  : NULL
REMARK   3     B13 (A**2)  : NULL
REMARK   3     B23 (A**2)  : NULL
REMARK   3
REMARK   3   ESTIMATED COORDINATE ERROR.
REMARK   3    ESD FROM LUZZATI PLOT       (A) : NULL
REMARK   3    ESD FROM SIGMAA             (A) : NULL
REMARK   3    LOW RESOLUTION CUTOFF       (A) : NULL
REMARK   3
REMARK   3   CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3    ESD FROM C-V LUZZATI PLOT   (A) : NULL
REMARK   3    ESD FROM C-V SIGMAA         (A) : NULL
REMARK   3
REMARK   3   RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3    BOND LENGTHS               (A) : 0.016
REMARK   3    BOND ANGLES           (DEGREES) : 2.5
REMARK   3    DIHEDRAL ANGLES       (DEGREES) : 22.8
REMARK   3    IMPROPER ANGLES       (DEGREES) : 2.05
REMARK   3
REMARK   3   ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK   3
REMARK   3   ISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS      SIGMA
REMARK   3    MAIN-CHAIN BOND            (A**2) : 1.2   ; 1.5
REMARK   3    MAIN-CHAIN ANGLE           (A**2) : 1.6   ; 2.0
REMARK   3    SIDE-CHAIN BOND            (A**2) : 2.1   ; 2.0
REMARK   3    SIDE-CHAIN ANGLE           (A**2) : 2.4   ; 2.5
REMARK   3
REMARK   3   NCS MODEL : RESTRAINTS
REMARK   3
REMARK   3   NCS RESTRAINTS.                          RMS    SIGMA/WEIGHT
REMARK   3    GROUP  1  POSITIONAL         (A) : NULL  ; NULL
REMARK   3    GROUP  1  B-FACTOR         (A**2) : NULL  ; NULL
REMARK   3
REMARK   3   PARAMETER FILE  1  : PARAM19_MOD.PRO
REMARK   3   PARAMETER FILE  2  : PARAM19.SOL
REMARK   3   PARAMETER FILE  3  : HETEROPARAM19.PAR
REMARK   3   TOPOLOGY FILE  1  : TOPH19_MOD.PRO
REMARK   3   TOPOLOGY FILE  2  : TOPH19.SOL
REMARK   3   TOPOLOGY FILE  3  : HETERO.TOP
REMARK   3
REMARK   3   OTHER REFINEMENT REMARKS: REFINEMENT WAS PERFORMED WITH
REMARK   3   ANOMALOUS ON; PARAM19_MOD.PRO AND TOPH19_MOD.PRO ARE
REMARK   3   MODIFIED PARAMETER AND TOPOLOGY FILES OF PARAM19.PRO AND
REMARK   3   TOPH19.PRO, RESPECTIVELY, FOR SELENOMETHIONYL PROTEINS.
REMARK   3   NCS RESTRAINTS WERE APPLIED ONLY DURING THE INITIAL
REMARK   3   REFINEMENT.
REMARK   4
REMARK   4   1SCF COMPLIES WITH FORMAT V. 2.3,
```

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FIGURE 8A-3

```
REMARK    6
REMARK    6 THE FOLLOWING RESIDUES ARE DISORDERED IN THE STRUCTURE:
REMARK    6 A1-10; A92-103; B1-10; B130-136; B139-141; C1-10; C92-103;
REMARK    6 C127-141; D1-10; D91-103; D128-141
REMARK    7
REMARK    7 THE SIDE CHAINS OF THE FOLLOWING RESIDUES ARE DISORDERED IN
REMARK    7 THE STRUCTURE: A11-13,A91,A127,A133,B11,B13,B93,B96-97,
REMARK    7 B103,B128,B137,C11,C13,C39,D11,D13,D90,D106,D127
REMARK    8
REMARK    8 LYS A 91 IS LAST RESIDUE BEFORE GAP, PHE B 129 IS LAST
REMARK    8 RESIDUE BEFORE GAP, LYS C 91 IS LAST RESIDUE BEFORE GAP,
REMARK    8 PHE C 126 IS LAST RESIDUE BEFORE GAP, VAL D 90 IS LAST
REMARK    8 RESIDUE BEFORE GAP.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200   EXPERIMENT TYPE                    : X-RAY DIFFRACTION
REMARK 200   DATE OF DATA COLLECTION            :
REMARK 200   TEMPERATURE            (KELVIN)    : 110
REMARK 200   PH                                 : 7.4
REMARK 200   NUMBER OF CRYSTALS USED            : 1
REMARK 200
REMARK 200   SYNCHROTRON            (Y/N)       : Y
REMARK 200   RADIATION SOURCE                   : NSLS
REMARK 200   BEAMLINE                           : X4A
REMARK 200   X-RAY GENERATOR MODEL              : NULL
REMARK 200   MONOCHROMATIC OR LAUE  (M/L)       : M
REMARK 200   WAVELENGTH OR RANGE       (A)      : 0.986
REMARK 200   MONOCHROMATOR                      : SILICON CRYSTAL
REMARK 200   OPTICS                             : MIRRORS
REMARK 200
REMARK 200   DETECTOR TYPE                      : IMAGE PLATE
REMARK 200   DETECTOR MANUFACTURER              : FUJI
REMARK 200   INTENSITY-INTEGRATION SOFTWARE     : DENSO
REMARK 200   DATA SCALING SOFTWARE              : SCALEPACK
REMARK 200
REMARK 200   NUMBER OF UNIQUE REFLECTIONS       : 65689
REMARK 200   RESOLUTION RANGE HIGH     (A)      : 2.0
REMARK 200   RESOLUTION RANGE LOW      (A)      : 25
REMARK 200   REJECTION CRITERIA  (SIGMA(I))     : -3
REMARK 200
REMARK 200 OVERALL.
REMARK 200   COMPLETENESS FOR RANGE    (%)      : 94.9
REMARK 200   DATA REDUNDANCY                    : 2.75
REMARK 200   R MERGE                   (I)      : NULL
REMARK 200   R SYM                     (I)      : 0.056
REMARK 200   <I/SIGMA(I)> FOR THE DATA SET      : 15.3
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200   HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.0
REMARK 200   HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.07
REMARK 200   COMPLETENESS FOR SHELL    (%)      : 72
REMARK 200   DATA REDUNDANCY IN SHELL           : 2.23
REMARK 200   R MERGE FOR SHELL         (I)      : NULL
REMARK 200   R SYM FOR SHELL           (I)      : 0.581
REMARK 200   <I/SIGMA(I)> FOR SHELL             : 1.6
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: NULL
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: MADLSQ
REMARK 200 STARTING MODEL: NULL
```

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FIGURE 8A-4

```
REMARK 200
REMARK 200  REMARK: NULL
REMARK 280
REMARK 280  CRYSTAL
REMARK 280  SOLVENT CONTENT, VS   (%): NULL
REMARK 280  MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280  CRYSTALLIZATION CONDITIONS: PROTEIN WAS CRYSTALLIZED FROM
REMARK 280  22% PEG 400, 220 MM CACL2, 100 MM HEPES, PH 7.4 AND 5MM
REMARK 280  DTT IN 20 DEGREE ROOM
REMARK 290
REMARK 290  CRYSTALLOGRAPHIC SYMMETRY
REMARK 290  SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21
REMARK 290
REMARK 290      SYMOP    SYMMETRY
REMARK 290      NNNMMM   OPERATOR
REMARK 290      1555     X,Y,Z
REMARK 290      2555     1/2-X,-Y,1/2+Z
REMARK 290      3555     -X,1/2+Y,1/2-Z
REMARK 290      4555     1/2+X,1/2-Y,-Z
REMARK 290
REMARK 290      WHERE NNN -> OPERATOR NUMBER
REMARK 290            MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290  CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290  THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290  RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290  RELATED MOLECULES.
REMARK 290      SMTRY1   1   1.000000   0.000000   0.000000        0.00000
REMARK 290      SMTRY2   1   0.000000   1.000000   0.000000        0.00000
REMARK 290      SMTRY3   1   0.000000   0.000000   1.000000        0.00000
REMARK 290      SMTRY1   2  -1.000000   0.000000   0.000000       35.90922
REMARK 290      SMTRY2   2   0.000000  -1.000000   0.000000        0.00000
REMARK 290      SMTRY3   2   0.000000   0.000000   1.000000       44.09560
REMARK 290      SMTRY1   3  -1.000000   0.000000   0.000000        0.00000
REMARK 290      SMTRY2   3   0.000000   1.000000   0.000000       41.27456
REMARK 290      SMTRY3   3   0.000000   0.000000  -1.000000       44.09560
REMARK 290      SMTRY1   4   1.000000   0.000000   0.000000       35.90922
REMARK 290      SMTRY2   4   0.000000  -1.000000   0.000000       41.27456
REMARK 290      SMTRY3   4   0.000000   0.000000  -1.000000        0.00000
REMARK 290
REMARK 290  REMARK: NULL
REMARK 295
REMARK 295  NON-CRYSTALLOGRAPHIC SYMMETRY
REMARK 295  THE TRANSFORMATIONS PRESENTED ON THE MTRIX RECORDS BELOW
REMARK 295  DESCRIBE NON-CRYSTALLOGRAPHIC RELATIONSHIPS AMONG ATOMS
REMARK 295  IN THIS ENTRY.  APPLYING THE APPROPRIATE MTRIX
REMARK 295  TRANSFORMATION TO THE RESIDUES LISTED FIRST WILL YIELD
REMARK 295  APPROXIMATE COORDINATES FOR THE RESIDUES LISTED SECOND.
REMARK 295  CHAIN IDENTIFIERS GIVEN AS "?" REFER TO CHAINS FOR WHICH
REMARK 295  ATOMS ARE NOT FOUND IN THIS ENTRY.
REMARK 295
REMARK 295                  APPLIED TO           TRANSFORMED TO
REMARK 295      TRANSFORM CHAIN   RESIDUES       CHAIN   RESIDUES       RMSD
REMARK 295        SSS
REMARK 295      M  1       B    11 .. 91          A    11 .. 91       1.020
REMARK 295      M  2       A    11 .. 91          C    11 .. 91       1.677
REMARK 295      M  3       D    11 .. 91          A    11 .. 91       1.926
REMARK 295      M  4       C    11 .. 91          B    11 .. 91       0.620
REMARK 295      M  5       D    11 .. 91          B    11 .. 91       1.764
```

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FIGURE 8A-5

```
REMARK 295      M  6         D  11 .. 91          C   11 .. 91      1.810
REMARK 295      M  7         C  11 .. 91          A   11 .. 91      0.898
REMARK 295
REMARK 295      WHERE SSS -> COLUMNS 8-10 OF MTRIX RECORDS
REMARK 295
REMARK 295 REMARK:
REMARK 295 TRANSFORMATION RELATES CHAIN B TO CHAIN A; INCLUDING
REMARK 295  RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN C TO CHAIN A; INCLUDING
REMARK 295  RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN D TO CHAIN A; INCLUDING
REMARK 295  RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN C TO CHAIN B; INCLUDING
REMARK 295  RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN D TO CHAIN B; INCLUDING
REMARK 295  RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN D TO CHAIN C; INCLUDING
REMARK 295  RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN CD DIMER TO CHAIN AB DIMER;
REMARK 295  INCLUDING RESIDUES A11-91,A104-126,B11-B90,B104-127,
REMARK 295  C11-91,C104-126,D11-90,D104-127
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470    M RES CSSEQI   ATOMS
REMARK 470      ASN A  11     CG    OD1   ND2
REMARK 470      VAL A  12     CG1   CG2
REMARK 470      LYS A  13     CG    CD    CE    NZ
REMARK 470      LYS A  91     CG    CD    CE    NZ
REMARK 470      LYS A 127     CG    CD    CE    NZ
REMARK 470      SER A 133     OG
REMARK 470      ASN B  11     CG    OD1   ND2
REMARK 470      LYS B  13     CG    CD    CE    NZ
REMARK 470      ASN B  93     CG    OD1   ND2
REMARK 470      LYS B  96     CG    CD    CE    NZ
REMARK 470      ASP B  97     CG    OD1   OD2
REMARK 470      LYS B 103     CG    CD    CE    NZ
REMARK 470      ASP B 128     CG    OD1   OD2
REMARK 470      ASP B 137  .  CG    OD1   OD2
REMARK 470      ASN C  11     CG    OD1   ND2
REMARK 470      LYS C  13     CG    CD    CE    NZ
REMARK 470      LEU C  39     CG    CD1   CD2
REMARK 470      ASN D  11     CG    OD1   ND2
REMARK 470      LYS D  13     CG    CD    CE    NZ
REMARK 470      VAL D  90     CG1   CG2
REMARK 470      GLU D 106     CG    CD    OE1   OE2
REMARK 470      LYS D 127     CG    CD    CE    NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS
REMARK 500
REMARK 500 THE FOLLOWING ATOMS THAT ARE RELATED BY CRYSTALLOGRAPHIC
REMARK 500 SYMMETRY ARE IN CLOSE CONTACT.  AN ATOM LOCATED WITHIN 0.15
REMARK 500 ANGSTROMS OF A SYMMETRY RELATED ATOM IS ASSUMED TO BE ON A
REMARK 500 SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375
REMARK 500 INSTEAD OF REMARK 500.  ATOMS WITH NON-BLANK ALTERNATE
REMARK 500 LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.
REMARK 500
```

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FIGURE 8A-6

```
REMARK 500 DISTANCE CUTOFF:
REMARK 500 2.2 ANGSTROMS FOR CONTACTS NOT INVOLVING HYDROGEN ATOMS
REMARK 500 1.6 ANGSTROMS FOR CONTACTS INVOLVING HYDROGEN ATOMS
REMARK 500
REMARK 500    ATM1  RES C  SSEQI   ATM2  RES C  SSEQI   SSYMOP   DISTANCE
REMARK 500    CA    CA    1021     O     VAL A  139      3655     2.18
REMARK 500
REMARK 500 REMARK: NULL
REMARK 600
REMARK 600 HETEROGEN
REMARK 600  1PE: ONLY PART OF THE PEG400 CHAIN IS ORDERED IN THE
REMARK 600  STRUCTURE.
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 1SCF  A    SWS    P21583      1 -   35 NOT IN ATOMS LIST
REMARK 999 1SCF  A    SWS    P21583    167 -  273 NOT IN ATOMS LIST
REMARK 999 1SCF  B    SWS    P21583      1 -   35 NOT IN ATOMS LIST
REMARK 999 1SCF  B    SWS    P21583    164 -  273 NOT IN ATOMS LIST
REMARK 999 1SCF  C    SWS    P21583      1 -   35 NOT IN ATOMS LIST
REMARK 999 1SCF  C    SWS    P21583    152 -  273 NOT IN ATOMS LIST
REMARK 999 1SCF  D    SWS    P21583      1 -   35 NOT IN ATOMS LIST
REMARK 999 1SCF  D    SWS    P21583    153 -  273 NOT IN ATOMS LIST
DBREF  1SCF A   11    91 SWS    P21583   SCF_HUMAN       36    116
DBREF  1SCF A  104   141 SWS    P21583   SCF_HUMAN      129    166
DBREF  1SCF B   11   129 SWS    P21583   SCF_HUMAN       36    154
DBREF  1SCF B  137   138 SWS    P21583   SCF_HUMAN      162    163
DBREF  1SCF C   11    91 SWS    P21583   SCF_HUMAN       36    116
DBREF  1SCF C  104   126 SWS    P21583   SCF_HUMAN      129    151
DBREF  1SCF D   11    90 SWS    P21583   SCF_HUMAN       36    115
DBREF  1SCF D  104   127 SWS    P21583   SCF_HUMAN      129    152
SEQADV 1SCF MSE A   27 SWS  P21583    MET    52 MODIFIED
SEQADV 1SCF MSE A   36 SWS  P21583    MET    61 MODIFIED
SEQADV 1SCF MSE A   48 SWS  P21583    MET    73 MODIFIED
SEQADV 1SCF     A      SWS  P21583    GLU   117 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    ASN   118 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    SER   119 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    SER   120 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    LYS   121 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    ASP   122 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    LEU   123 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    LYS   124 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    LYS   125 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    SER   126 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    PHE   127 GAP IN PDB ENTRY
SEQADV 1SCF     A      SWS  P21583    LYS   128 GAP IN PDB ENTRY
SEQADV 1SCF MSE B   27 SWS  P21583    MET    52 MODIFIED
SEQADV 1SCF MSE B   36 SWS  P21583    MET    61 MODIFIED
SEQADV 1SCF MSE B   48 SWS  P21583    MET    73 MODIFIED
SEQADV 1SCF     B      SWS  P21583    VAL   155 GAP IN PDB ENTRY
SEQADV 1SCF     B      SWS  P21583    VAL   156 GAP IN PDB ENTRY
SEQADV 1SCF     B      SWS  P21583    ALA   157 GAP IN PDB ENTRY
SEQADV 1SCF     B      SWS  P21583    SER   158 GAP IN PDB ENTRY
SEQADV 1SCF     B      SWS  P21583    GLU   159 GAP IN PDB ENTRY
SEQADV 1SCF     B      SWS  P21583    THR   160 GAP IN PDB ENTRY
SEQADV 1SCF     B      SWS  P21583    SER   161 GAP IN PDB ENTRY
SEQADV 1SCF MSE C   27 SWS  P21583    MET    52 MODIFIED
SEQADV 1SCF MSE C   36 SWS  P21583    MET    61 MODIFIED
SEQADV 1SCF MSE C   48 SWS  P21583    MET    73 MODIFIED
SEQADV 1SCF     C      SWS  P21583    GLU   117 GAP IN PDB ENTRY
SEQADV 1SCF     C      SWS  P21583    ASN   118 GAP IN PDB ENTRY
```

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FIGURE 8A-7

```
SEQADV 1SCF        C        SWS  P21583   SER   119 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   SER   120 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   LYS   121 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   ASP   122 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   LEU   123 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   LYS   124 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   LYS   125 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   SER   126 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   PHE   127 GAP IN PDB ENTRY
SEQADV 1SCF        C        SWS  P21583   LYS   128 GAP IN PDB ENTRY
SEQADV 1SCF MSE D  27       SWS  P21583   MET    52 MODIFIED
SEQADV 1SCF MSE D  36       SWS  P21583   MET    61 MODIFIED
SEQADV 1SCF MSE D  48       SWS  P21583   MET    73 MODIFIED
SEQADV 1SCF        D        SWS  P21583   LYS   116 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   GLU   117 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   ASN   118 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   SER   119 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   SER   120 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   LYS   121 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   ASP   122 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   LEU   123 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   LYS   124 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   LYS   125 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   SER   126 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   PHE   127 GAP IN PDB ENTRY
SEQADV 1SCF        D        SWS  P21583   LYS   128 GAP IN PDB ENTRY
SEQRES    1 A  273  MET LYS LYS THR GLN THR TRP ILE LEU THR CYS ILE TYR
SEQRES    2 A  273  LEU GLN LEU LEU LEU PHE ASN PRO LEU VAL LYS THR GLU
SEQRES    3 A  273  GLY ILE CYS ARG ASN ARG VAL THR ASN ASN VAL LYS ASP
SEQRES    4 A  273  VAL THR LYS LEU VAL ALA ASN LEU PRO LYS ASP TYR MSE
SEQRES    5 A  273  ILE THR LEU LYS TYR VAL PRO GLY MSE ASP VAL LEU PRO
SEQRES    6 A  273  SER HIS CYS TRP ILE SER GLU MSE VAL VAL GLN LEU SER
SEQRES    7 A  273  ASP SER LEU THR ASP LEU LEU ASP LYS PHE SER ASN ILE
SEQRES    8 A  273  SER GLU GLY LEU SER ASN TYR SER ILE ILE ASP LYS LEU
SEQRES    9 A  273  VAL ASN ILE VAL ASP ASP LEU VAL GLU CYS VAL LYS GLU
SEQRES   10 A  273  ASN SER SER LYS ASP LEU LYS LYS SER PHE LYS SER PRO
SEQRES   11 A  273  GLU PRO ARG LEU PHE THR PRO GLU GLU PHE PHE ARG ILE
SEQRES   12 A  273  PHE ASN ARG SER ILE ASP ALA PHE LYS ASP PHE VAL VAL
SEQRES   13 A  273  ALA SER GLU THR SER ASP CYS VAL VAL SER SER THR LEU
SEQRES   14 A  273  SER PRO GLU LYS ASP SER ARG VAL SER VAL THR LYS PRO
SEQRES   15 A  273  PHE MET LEU PRO PRO VAL ALA ALA SER SER LEU ARG ASN
SEQRES   16 A  273  ASP SER SER SER SER ASN ARG LYS ALA LYS ASN PRO PRO
SEQRES   17 A  273  GLY ASP SER SER LEU HIS TRP ALA ALA MET ALA LEU PRO
SEQRES   18 A  273  ALA LEU PHE SER LEU ILE ILE GLY PHE ALA PHE GLY ALA
SEQRES   19 A  273  LEU TYR TRP LYS LYS ARG GLN PRO SER LEU THR ARG ALA
SEQRES   20 A  273  VAL GLU ASN ILE GLN ILE ASN GLU GLU ASP ASN GLU ILE
SEQRES   21 A  273  SER MET LEU GLN GLU LYS GLU ARG GLU PHE GLN GLU VAL
SEQRES    1 B  273  MET LYS LYS THR GLN THR TRP ILE LEU THR CYS ILE TYR
SEQRES    2 B  273  LEU GLN LEU LEU LEU PHE ASN PRO LEU VAL LYS THR GLU
SEQRES    3 B  273  GLY ILE CYS ARG ASN ARG VAL THR ASN ASN VAL LYS ASP
SEQRES    4 B  273  VAL THR LYS LEU VAL ALA ASN LEU PRO LYS ASP TYR MSE
SEQRES    5 B  273  ILE THR LEU LYS TYR VAL PRO GLY MSE ASP VAL LEU PRO
SEQRES    6 B  273  SER HIS CYS TRP ILE SER GLU MSE VAL VAL GLN LEU SER
SEQRES    7 B  273  ASP SER LEU THR ASP LEU LEU ASP LYS PHE SER ASN ILE
SEQRES    8 B  273  SER GLU GLY LEU SER ASN TYR SER ILE ILE ASP LYS LEU
SEQRES    9 B  273  VAL ASN ILE VAL ASP ASP LEU VAL GLU CYS VAL LYS GLU
SEQRES   10 B  273  ASN SER SER LYS ASP LEU LYS LYS SER PHE LYS SER PRO
SEQRES   11 B  273  GLU PRO ARG LEU PHE THR PRO GLU GLU PHE PHE ARG ILE
SEQRES   12 B  273  PHE ASN ARG SER ILE ASP ALA PHE LYS ASP PHE VAL VAL
SEQRES   13 B  273  ALA SER GLU THR SER ASP CYS VAL VAL SER SER THR LEU
```

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FIGURE 8A-8

```
SEQRES   14 B   273    SER PRO GLU LYS ASP SER ARG VAL SER VAL THR LYS PRO
SEQRES   15 B   273    PHE MET LEU PRO PRO VAL ALA ALA SER SER LEU ARG ASN
SEQRES   16 B   273    ASP SER SER SER SER ASN ARG LYS ALA LYS ASN PRO PRO
SEQRES   17 B   273    GLY ASP SER SER LEU HIS TRP ALA ALA MET ALA LEU PRO
SEQRES   18 B   273    ALA LEU PHE SER LEU ILE ILE GLY PHE ALA PHE GLY ALA
SEQRES   19 B   273    LEU TYR TRP LYS LYS ARG GLN PRO SER LEU THR ARG ALA
SEQRES   20 B   273    VAL GLU ASN ILE GLN ILE ASN GLU GLU ASP ASN GLU ILE
SEQRES   21 B   273    SER MET LEU GLN GLU LYS GLU ARG GLU PHE GLN GLU VAL
SEQRES    1 C   273    MET LYS LYS THR GLN THR TRP ILE LEU THR CYS ILE TYR
SEQRES    2 C   273    LEU GLN LEU LEU LEU PHE ASN PRO LEU VAL LYS THR GLU
SEQRES    3 C   273    GLY ILE CYS ARG ASN ARG VAL THR ASN ASN VAL LYS ASP
SEQRES    4 C   273    VAL THR LYS LEU VAL ALA ASN LEU PRO LYS ASP TYR MSE
SEQRES    5 C   273    ILE THR LEU LYS TYR VAL PRO GLY MSE ASP VAL LEU PRO
SEQRES    6 C   273    SER HIS CYS TRP ILE SER GLU MSE VAL VAL GLN LEU SER
SEQRES    7 C   273    ASP SER LEU THR ASP LEU LEU ASP LYS PHE SER ASN ILE
SEQRES    8 C   273    SER GLU GLY LEU SER ASN TYR SER ILE ILE ASP LYS LEU
SEQRES    9 C   273    VAL ASN ILE VAL ASP ASP LEU VAL GLU CYS VAL LYS GLU
SEQRES   10 C   273    ASN SER SER LYS ASP LEU LYS LYS SER PHE LYS SER PRO
SEQRES   11 C   273    GLU PRO ARG LEU PHE THR PRO GLU GLU PHE PHE ARG ILE
SEQRES   12 C   273    PHE ASN ARG SER ILE ASP ALA PHE LYS ASP PHE VAL VAL
SEQRES   13 C   273    ALA SER GLU THR SER ASP CYS VAL VAL SER SER THR LEU
SEQRES   14 C   273    SER PRO GLU LYS ASP SER ARG VAL SER VAL THR LYS PRO
SEQRES   15 C   273    PHE MET LEU PRO PRO VAL ALA ALA SER SER LEU ARG ASN
SEQRES   16 C   273    ASP SER SER SER SER ASN ARG LYS ALA LYS ASN PRO PRO
SEQRES   17 C   273    GLY ASP SER SER LEU HIS TRP ALA ALA MET ALA LEU PRO
SEQRES   18 C   273    ALA LEU PHE SER LEU ILE ILE GLY PHE ALA PHE GLY ALA
SEQRES   19 C   273    LEU TYR TRP LYS LYS ARG GLN PRO SER LEU THR ARG ALA
SEQRES   20 C   273    VAL GLU ASN ILE GLN ILE ASN GLU GLU ASP ASN GLU ILE
SEQRES   21 C   273    SER MET LEU GLN GLU LYS GLU ARG GLU PHE GLN GLU VAL
SEQRES    1 D   273    MET LYS LYS THR GLN THR TRP ILE LEU THR CYS ILE TYR
SEQRES    2 D   273    LEU GLN LEU LEU LEU PHE ASN PRO LEU VAL LYS THR GLU
SEQRES    3 D   273    GLY ILE CYS ARG ASN ARG VAL THR ASN ASN VAL LYS ASP
SEQRES    4 D   273    VAL THR LYS LEU VAL ALA ASN LEU PRO LYS ASP TYR MSE
SEQRES    5 D   273    ILE THR LEU LYS TYR VAL PRO GLY MSE ASP VAL LEU PRO
SEQRES    6 D   273    SER HIS CYS TRP ILE SER GLU MSE VAL VAL GLN LEU SER
SEQRES    7 D   273    ASP SER LEU THR ASP LEU LEU ASP LYS PHE SER ASN ILE
SEQRES    8 D   273    SER GLU GLY LEU SER ASN TYR SER ILE ILE ASP LYS LEU
SEQRES    9 D   273    VAL ASN ILE VAL ASP ASP LEU VAL GLU CYS VAL LYS GLU
SEQRES   10 D   273    ASN SER SER LYS ASP LEU LYS LYS SER PHE LYS SER PRO
SEQRES   11 D   273    GLU PRO ARG LEU PHE THR PRO GLU GLU PHE PHE ARG ILE
SEQRES   12 D   273    PHE ASN ARG SER ILE ASP ALA PHE LYS ASP PHE VAL VAL
SEQRES   13 D   273    ALA SER GLU THR SER ASP CYS VAL VAL SER SER THR LEU
SEQRES   14 D   273    SER PRO GLU LYS ASP SER ARG VAL SER VAL THR LYS PRO
SEQRES   15 D   273    PHE MET LEU PRO PRO VAL ALA ALA SER SER LEU ARG ASN
SEQRES   16 D   273    ASP SER SER SER SER ASN ARG LYS ALA LYS ASN PRO PRO
SEQRES   17 D   273    GLY ASP SER SER LEU HIS TRP ALA ALA MET ALA LEU PRO
SEQRES   18 D   273    ALA LEU PHE SER LEU ILE ILE GLY PHE ALA PHE GLY ALA
SEQRES   19 D   273    LEU TYR TRP LYS LYS ARG GLN PRO SER LEU THR ARG ALA
SEQRES   20 D   273    VAL GLU ASN ILE GLN ILE ASN GLU GLU ASP ASN GLU ILE
SEQRES   21 D   273    SER MET LEU GLN GLU LYS GLU ARG GLU PHE GLN GLU VAL
MODRES 1SCF MSE A    27    MET    SELENOMETHIONINE
MODRES 1SCF MSE A    36    MET    SELENOMETHIONINE
MODRES 1SCF MSE A    48    MET    SELENOMETHIONINE
MODRES 1SCF MSE B    27    MET    SELENOMETHIONINE
MODRES 1SCF MSE B    36    MET    SELENOMETHIONINE
MODRES 1SCF MSE B    48    MET    SELENOMETHIONINE
MODRES 1SCF MSE C    27    MET    SELENOMETHIONINE
MODRES 1SCF MSE C    36    MET    SELENOMETHIONINE
MODRES 1SCF MSE C    48    MET    SELENOMETHIONINE
MODRES 1SCF MSE D    27    MET    SELENOMETHIONINE
```

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FIGURE 8A-9

```
MODRES 1SCF MSE D    36   MET   SELENOMETHIONINE
MODRES 1SCF MSE D    48   MET   SELENOMETHIONINE
HET      MSE  A  27        8
HET      MSE  A  36        8
HET      MSE  A  48        8
HET      MSE  B  27        8
HET      MSE  B  36        8
HET      MSE  B  48        8
HET      MSE  C  27        8
HET      MSE  C  36        8
HET      MSE  C  48        8
HET      MSE  D  27        8
HET      MSE  D  36        8
HET      MSE  D  48        8
HET      CA   1021        1
HET      CA   1022        1
HET      CA   1023        1
HET      1PE       1      16
HETNAM      MSE SELENOMETHIONINE
HETNAM      CA  CALCIUM ION
HETNAM      1PE POLYETHYLENE GLYCOL
HETSYN      1PE PEG400
FORMUL   1  MSE      3(C5 H11 N1 O2 SE1)
FORMUL   2  MSE      3(C5 H11 N1 O2 SE1)
FORMUL   3  MSE      3(C5 H11 N1 O2 SE1)
FORMUL   4  MSE      3(C5 H11 N1 O2 SE1)
FORMUL   5  CA       3(CA1 2+)
FORMUL   6  1PE      C10 H22 O6
FORMUL   7  HOH     *264(H2 O1)
HELIX    1   1 VAL A   12  ASN A   21  1                        10
HELIX    2   2 SER A   41  CYS A   43  5                         3
HELIX    3   3 SER A   46  LYS A   62  5                        17
HELIX    4   4 ASN A   72  CYS A   89  1                        18
HELIX    5   5 PRO A  112  LYS A  127  1                        16
HELIX    6   6 VAL B   12  ASN B   21  1                        10
HELIX    7   7 SER B   41  CYS B   43  5                         3
HELIX    8   8 SER B   46  LYS B   62  5                        17
HELIX    9   9 ASN B   72  GLU B   92  1                        21
HELIX   10  10 PRO B  112  LYS B  127  1                        16
HELIX   11  11 VAL C   12  ASN C   21  1                        10
HELIX   12  12 SER C   41  LYS C   62  1                        22
HELIX   13  13 ASN C   72  VAL C   90  1                        19
HELIX   14  14 PRO C  112  ASP C  124  1                        13
HELIX   15  15 VAL D   12  ASN D   21  1                        10
HELIX   16  16 SER D   41  CYS D   43  5                         3
HELIX   17  17 SER D   46  LYS D   62  5                        17
HELIX   18  18 ASN D   72  CYS D   89  1                        18
HELIX   19  19 PRO D  112  ALA D  125  1                        14
SHEET    1   A 2 THR A   29  LYS A   31  0
SHEET    2   A 2 PRO A  107  LEU A  109 -1  N  ARG A 108  O  LEU A  30
SHEET    1   B 2 THR B   29  LYS B   31  0
SHEET    2   B 2 PRO B  107  LEU B  109 -1  N  ARG B 108  O  LEU B  30
SHEET    1   C 2 THR C   29  LYS C   31  0
SHEET    2   C 2 PRO C  107  LEU C  109 -1  N  ARG C 108  O  LEU C  30
SHEET    1   D 2 THR D   29  LYS D   31  0
SHEET    2   D 2 PRO D  107  LEU D  109 -1  N  ARG D 108  O  LEU D  30
SSBOND   1 CYS A   43    CYS A  138
SSBOND   2 CYS B   43    CYS B  138
LINK        .   N   MSE A   27             C   TYR A  26
LINK        .   C   MSE A   27             N   ILE A  28
```

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FIGURE 8A-10

LINK		N	MSE	A	36	C	GLY A	35
LINK		C	MSE	A	36	N	ASP A	37
LINK		N	MSE	A	48	C	GLU A	47
LINK		C	MSE	A	48	N	VAL A	49
LINK		N	MSE	B	27	C	TYR B	26
LINK		C	MSE	B	27	N	ILE B	28
LINK		N	MSE	B	36	C	GLY B	35
LINK		C	MSE	B	36	N	ASP B	37
LINK		N	MSE	B	48	C	GLU B	47
LINK		C	MSE	B	48	N	VAL B	49
LINK		N	MSE	C	27	C	TYR C	26
LINK		C	MSE	C	27	N	ILE C	28
LINK		N	MSE	C	36	C	GLY C	35
LINK		C	MSE	C	36	N	ASP C	37
LINK		N	MSE	C	48	C	GLU C	47
LINK		C	MSE	C	48	N	VAL C	49
LINK		N	MSE	D	27	C	TYR D	26
LINK		C	MSE	D	27	N	ILE D	28
LINK		N	MSE	D	36	C	GLY D	35
LINK		C	MSE	D	36	N	ASP D	37
LINK		N	MSE	D	48	C	GLU D	47
LINK		C	MSE	D	48	N	VAL D	49
LINK		CA	CA		1021	O	HOH	1024
LINK		CA	CA		1021	O	HOH	1025
LINK		CA	CA		1023	O	HOH	1027
LINK		CA	CA		1023	O	HOH	1028
LINK		CA	CA		1023	O	HOH	1029

```
CISPEP   1 SER A  104      PRO A  105                O         -0.10
CRYST1   71.820    82.550    88.190   90.00   90.00   90.00 P 21 21 21      4
ORIGX1      1.000000  0.000000  0.000000            0.00000
ORIGX2      0.000000  1.000000  0.000000            0.00000
ORIGX3      0.000000  0.000000  1.000000            0.00000
SCALE1      0.013924  0.000000  0.000000            0.00000
SCALE2      0.000000  0.012114  0.000000            0.00000
SCALE3      0.000000  0.000000  0.011339            0.00000
MTRIX1   1  0.915300  0.368400  0.162800          -10.34380       1
MTRIX2   1  0.357100 -0.929200  0.095000           35.55670       1
MTRIX3   1  0.186300 -0.028800 -0.982100           43.17570       1
MTRIX1   2 -0.935658 -0.315827 -0.157471           63.79985       1
MTRIX2   2 -0.265278  0.923709 -0.276386           17.94411       1
MTRIX3   2  0.232747 -0.216829 -0.948058           63.68074       1
MTRIX1   3 -0.994700  0.088300 -0.051700           54.54720       1
MTRIX2   3 -0.094000 -0.988400  0.119100           48.88150       1
MTRIX3   3 -0.040600  0.123400  0.991500          -20.54390       1
MTRIX1   4 -0.991100  0.100500 -0.087800           55.16840       1
MTRIX2   4 -0.117800 -0.968000  0.221700           45.07210       1
MTRIX3   4 -0.062700  0.230100  0.971100          -21.92400       1
MTRIX1   5 -0.951900 -0.248300  0.179700           52.26270       1
MTRIX2   5 -0.277100  0.947600 -0.158800           13.33780       1
MTRIX3   5 -0.130900 -0.200900 -0.970800           74.41510       1
MTRIX1   6  0.984200  0.147100 -0.098100            0.55340       1
MTRIX2   6  0.142600 -0.988400 -0.052100           52.60730       1
MTRIX3   6 -0.104600  0.037300 -0.993800           86.74100       1
MTRIX1   7 -0.955400 -0.244200  0.166100           52.84290       1
MTRIX2   7 -0.269500  0.950900 -0.152200           12.52990       1
MTRIX3   7 -0.120800 -0.190100 -0.974300           73.76110       1
ATOM     1  N   ASN A   11       10.232   3.110  20.636  1.00 60.07      N
ATOM     2  CA  ASN A   11        9.176   3.892  19.994  1.00 59.79      C
ATOM     3  C   ASN A   11        9.647   5.204  19.309  1.00 59.52      C
ATOM     4  O   ASN A   11        9.661   6.288  19.910  1.00 59.97      O
```

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FIGURE 8A-11

ATOM	5	CB	ASN	A	11	8.113	4.228	21.038	1.00	60.46	C
ATOM	6	N	VAL	A	12	10.013	5.143	18.009	1.00	57.40	N
ATOM	7	CA	VAL	A	12	10.715	6.225	17.309	1.00	53.71	C
ATOM	8	C	VAL	A	12	9.844	7.387	16.820	1.00	50.84	C
ATOM	9	O	VAL	A	12	10.343	8.268	16.130	1.00	51.46	O
ATOM	10	CB	VAL	A	12	11.541	5.657	16.126	1.00	53.25	C
ATOM	11	N	LYS	A	13	8.543	7.490	17.147	1.00	49.07	N
ATOM	12	CA	LYS	A	13	7.721	8.640	16.756	1.00	44.35	C
ATOM	13	C	LYS	A	13	8.114	9.879	17.542	1.00	42.88	C
ATOM	14	O	LYS	A	13	8.271	10.995	17.007	1.00	41.79	O
ATOM	15	CB	LYS	A	13	6.258	8.378	17.093	1.00	44.76	C
ATOM	16	N	ASP	A	14	8.283	9.557	18.839	1.00	38.29	N
ATOM	17	CA	ASP	A	14	8.609	10.545	19.818	1.00	35.56	C
ATOM	18	C	ASP	A	14	10.068	10.894	19.718	1.00	32.01	C
ATOM	19	O	ASP	A	14	10.389	12.060	19.896	1.00	30.80	O
ATOM	20	CB	ASP	A	14	8.151	10.072	21.200	1.00	38.77	C
ATOM	21	CG	ASP	A	14	6.725	10.518	21.630	1.00	43.77	C
ATOM	22	OD1	ASP	A	14	6.046	11.324	20.969	1.00	45.53	O
ATOM	23	OD2	ASP	A	14	6.269	10.057	22.680	1.00	47.33	O
ATOM	24	N	VAL	A	15	10.939	9.938	19.360	1.00	28.31	N
ATOM	25	CA	VAL	A	15	12.335	10.224	19.089	1.00	27.35	C
ATOM	26	C	VAL	A	15	12.510	11.219	17.959	1.00	29.06	C
ATOM	27	O	VAL	A	15	13.265	12.166	18.138	1.00	32.49	O
ATOM	28	CB	VAL	A	15	13.191	8.976	18.792	1.00	26.33	C
ATOM	29	CG1	VAL	A	15	14.623	9.347	18.405	1.00	20.32	C
ATOM	30	CG2	VAL	A	15	13.215	8.064	20.008	1.00	24.37	C
ATOM	31	N	THR	A	16	11.858	11.085	16.807	1.00	28.42	N
ATOM	32	CA	THR	A	16	11.968	12.085	15.758	1.00	27.97	C
ATOM	33	C	THR	A	16	11.386	13.413	16.208	1.00	25.43	C
ATOM	34	O	THR	A	16	12.020	14.418	15.905	1.00	25.82	O
ATOM	35	CB	THR	A	16	11.357	11.646	14.385	1.00	27.70	C
ATOM	36	OG1	THR	A	16	9.959	11.529	14.588	1.00	32.27	O
ATOM	37	CG2	THR	A	16	11.931	10.335	13.912	1.00	25.71	C
ATOM	38	N	LYS	A	17	10.243	13.459	16.928	1.00	24.83	N
ATOM	39	CA	LYS	A	17	9.701	14.698	17.482	1.00	23.60	C
ATOM	40	C	LYS	A	17	10.659	15.401	18.410	1.00	21.54	C
ATOM	41	O	LYS	A	17	10.756	16.624	18.373	1.00	23.88	O
ATOM	42	CB	LYS	A	17	8.365	14.488	18.206	1.00	27.08	C
ATOM	43	CG	LYS	A	17	7.291	14.120	17.198	1.00	34.84	C
ATOM	44	CD	LYS	A	17	5.881	14.040	17.781	1.00	40.64	C
ATOM	45	CE	LYS	A	17	4.800	13.911	16.665	1.00	45.98	C
ATOM	46	NZ	LYS	A	17	4.607	12.559	16.140	1.00	48.58	N
ATOM	47	N	LEU	A	18	11.417	14.646	19.212	1.00	19.73	N
ATOM	48	CA	LEU	A	18	12.377	15.207	20.151	1.00	17.98	C
ATOM	49	C	LEU	A	18	13.544	15.778	19.401	1.00	17.55	C
ATOM	50	O	LEU	A	18	13.813	16.959	19.523	1.00	17.68	O
ATOM	51	CB	LEU	A	18	12.875	14.144	21.121	1.00	17.63	C
ATOM	52	CG	LEU	A	18	13.850	14.582	22.216	1.00	15.34	C
ATOM	53	CD1	LEU	A	18	13.278	15.668	23.080	1.00	15.28	C
ATOM	54	CD2	LEU	A	18	14.253	13.389	23.032	1.00	14.40	C
ATOM	55	N	VAL	A	19	14.189	14.952	18.577	1.00	18.35	N
ATOM	56	CA	VAL	A	19	15.187	15.421	17.628	1.00	19.40	C
ATOM	57	C	VAL	A	19	14.757	16.628	16.824	1.00	18.97	C
ATOM	58	O	VAL	A	19	15.533	17.562	16.711	1.00	22.36	O
ATOM	59	CB	VAL	A	19	15.668	14.325	16.729	1.00	18.19	C
ATOM	60	CG1	VAL	A	19	16.675	14.817	15.708	1.00	20.68	C
ATOM	61	CG2	VAL	A	19	16.422	13.390	17.612	1.00	19.91	C
ATOM	62	N	ALA	A	20	13.530	16.732	16.366	1.00	18.27	N
ATOM	63	CA	ALA	A	20	13.105	17.946	15.719	1.00	17.82	C
ATOM	64	C	ALA	A	20	12.923	19.074	16.711	1.00	18.90	C

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FIGURE 8A-12

ATOM	65	O	ALA	A	20	12.977	20.244	16.352	1.00	20.70	O
ATOM	66	CB	ALA	A	20	11.777	17.661	15.059	1.00	17.70	C
ATOM	67	N	ASN	A	21	12.677	18.787	17.979	1.00	20.04	N
ATOM	68	CA	ASN	A	21	12.450	19.852	18.933	1.00	20.73	C
ATOM	69	C	ASN	A	21	13.695	20.161	19.771	1.00	20.34	C
ATOM	70	O	ASN	A	21	13.627	20.909	20.741	1.00	21.05	O
ATOM	71	CB	ASN	A	21	11.235	19.456	19.751	1.00	20.84	C
ATOM	72	CG	ASN	A	21	10.409	20.664	20.103	1.00	21.87	C
ATOM	73	OD1	ASN	A	21	10.157	21.501	19.250	1.00	20.51	O
ATOM	74	ND2	ASN	A	21	9.983	20.853	21.359	1.00	25.03	N
ATOM	75	N	LEU	A	22	14.851	19.615	19.399	1.00	18.22	N
ATOM	76	CA	LEU	A	22	16.129	19.924	20.000	1.00	17.27	C
ATOM	77	C	LEU	A	22	17.023	20.733	19.051	1.00	19.37	C
ATOM	78	O	LEU	A	22	17.001	20.468	17.851	1.00	19.69	O
ATOM	79	CB	LEU	A	22	16.856	18.631	20.432	1.00	16.17	C
ATOM	80	CG	LEU	A	22	16.342	17.790	21.598	1.00	14.77	C
ATOM	81	CD1	LEU	A	22	17.058	16.447	21.768	1.00	14.07	C
ATOM	82	CD2	LEU	A	22	16.463	18.606	22.862	1.00	11.82	C
ATOM	83	N	PRO	A	23	17.833	21.728	19.457	1.00	19.42	N
ATOM	84	CA	PRO	A	23	18.655	22.511	18.537	1.00	19.17	C
ATOM	85	C	PRO	A	23	19.694	21.621	17.878	1.00	20.53	C
ATOM	86	O	PRO	A	23	20.318	20.832	18.575	1.00	21.23	O
ATOM	87	CB	PRO	A	23	19.341	23.488	19.459	1.00	18.21	C
ATOM	88	CG	PRO	A	23	18.549	23.480	20.755	1.00	16.10	C
ATOM	89	CD	PRO	A	23	18.206	22.015	20.846	1.00	17.73	C
ATOM	90	N	LYS	A	24	19.959	21.716	16.571	1.00	23.65	N
ATOM	91	CA	LYS	A	24	20.937	20.852	15.866	1.00	27.23	C
ATOM	92	C	LYS	A	24	22.388	20.847	16.370	1.00	25.36	C
ATOM	93	O	LYS	A	24	23.179	19.918	16.149	1.00	25.16	O
ATOM	94	CB	LYS	A	24	20.931	21.150	14.332	1.00	29.02	C
ATOM	95	CG	LYS	A	24	19.550	20.939	13.680	1.00	36.19	C
ATOM	96	CD	LYS	A	24	19.557	21.512	12.245	1.00	43.22	C
ATOM	97	CE	LYS	A	24	18.207	21.800	11.585	1.00	42.88	C
ATOM	98	NZ	LYS	A	24	18.433	22.694	10.448	1.00	48.02	N
ATOM	99	N	ASP	A	25	22.712	21.900	17.110	1.00	26.32	N
ATOM	100	CA	ASP	A	25	24.060	22.087	17.653	1.00	28.70	C
ATOM	101	C	ASP	A	25	24.209	22.024	19.180	1.00	26.91	C
ATOM	102	O	ASP	A	25	25.225	22.386	19.785	1.00	27.43	O
ATOM	103	CB	ASP	A	25	24.551	23.433	17.144	1.00	30.59	C
ATOM	104	CG	ASP	A	25	23.780	24.615	17.684	1.00	33.09	C
ATOM	105	OD1	ASP	A	25	22.556	24.529	17.847	1.00	34.74	O
ATOM	106	OD2	ASP	A	25	24.421	25.638	17.933	1.00	37.53	O
ATOM	107	N	TYR	A	26	23.122	21.605	19.808	1.00	24.09	N
ATOM	108	CA	TYR	A	26	23.165	21.289	21.189	1.00	20.96	C
ATOM	109	C	TYR	A	26	23.821	19.937	21.246	1.00	20.04	C
ATOM	110	O	TYR	A	26	23.282	18.951	20.780	1.00	22.61	O
ATOM	111	CB	TYR	A	26	21.759	21.239	21.710	1.00	20.00	C
ATOM	112	CG	TYR	A	26	21.728	20.927	23.199	1.00	23.05	C
ATOM	113	CD1	TYR	A	26	22.430	21.764	24.039	1.00	20.56	C
ATOM	114	CD2	TYR	A	26	21.015	19.843	23.683	1.00	22.87	C
ATOM	115	CE1	TYR	A	26	22.421	21.541	25.376	1.00	23.76	C
ATOM	116	CE2	TYR	A	26	20.993	19.629	25.047	1.00	22.41	C
ATOM	117	CZ	TYR	A	26	21.693	20.493	25.877	1.00	23.68	C
ATOM	118	OH	TYR	A	26	21.661	20.353	27.259	1.00	22.67	O
HETATM	119	N	MSE	A	27	25.003	19.890	21.809	1.00	21.07	N
HETATM	120	CA	MSE	A	27	25.716	18.643	22.008	1.00	21.95	C
HETATM	121	C	MSE	A	27	25.325	17.906	23.296	1.00	23.63	C
HETATM	122	O	MSE	A	27	25.089	18.481	24.371	1.00	22.77	O
HETATM	123	CB	MSE	A	27	27.201	18.955	22.055	1.00	27.32	C
HETATM	124	CG	MSE	A	27	27.695	19.788	20.866	1.00	28.96	C

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FIGURE 8A-13

HETATM	125	SE	MSE A	27	27.207	18.877	19.234	1.00	37.24	SE
HETATM	126	CE	MSE A	27	28.489	17.511	19.371	1.00	26.83	C
ATOM	127	N	ILE A	28	25.250	16.576	23.165	1.00	22.91	N
ATOM	128	CA	ILE A	28	24.860	15.666	24.240	1.00	21.29	C
ATOM	129	C	ILE A	28	26.030	14.713	24.494	1.00	21.02	C
ATOM	130	O	ILE A	28	26.530	14.075	23.571	1.00	20.97	O
ATOM	131	CB	ILE A	28	23.550	14.901	23.870	1.00	19.78	C
ATOM	132	CG1	ILE A	28	22.372	15.818	23.534	1.00	17.37	C
ATOM	133	CG2	ILE A	28	23.147	14.006	25.006	1.00	18.93	C
ATOM	134	CD1	ILE A	28	21.207	15.120	22.805	1.00	16.08	C
ATOM	135	N	THR A	29	26.492	14.597	25.744	1.00	20.17	N
ATOM	136	CA	THR A	29	27.592	13.727	26.087	1.00	20.16	C
ATOM	137	C	THR A	29	27.065	12.315	26.319	1.00	20.21	
ATOM	138	O	THR A	29	26.051	12.081	26.988	1.00	19.29	
ATOM	139	CB	THR A	29	28.269	14.295	27.333	1.00	21.22	
ATOM	140	OG1	THR A	29	28.515	15.655	27.048	1.00	24.08	
ATOM	141	CG2	THR A	29	29.593	13.644	27.634	1.00	23.19	
ATOM	142	N	LEU A	30	27.767	11.369	25.708	1.00	18.56	
ATOM	143	CA	LEU A	30	27.462	9.976	25.862	1.00	17.76	C
ATOM	144	C	LEU A	30	28.824	9.351	25.959	1.00	18.41	C
ATOM	145	O	LEU A	30	29.738	9.774	25.283	1.00	20.72	C
ATOM	146	CB	LEU A	30	26.649	9.396	24.642	1.00	19.78	C
ATOM	147	CG	LEU A	30	26.350	7.884	24.473	1.00	14.53	N
ATOM	148	CD1	LEU A	30	25.475	7.478	25.601	1.00	18.04	C
ATOM	149	CD2	LEU A	30	25.629	7.525	23.205	1.00	14.92	C
ATOM	150	N	LYS A	31	28.984	8.378	26.833	1.00	18.64	O
ATOM	151	CA	LYS A	31	30.176	7.575	26.918	1.00	20.71	C
ATOM	152	C	LYS A	31	29.940	6.417	25.999	1.00	21.51	C
ATOM	153	O	LYS A	31	28.966	5.701	26.170	1.00	23.02	C
ATOM	154	CB	LYS A	31	30.411	7.009	28.295	1.00	19.63	N
ATOM	155	CG	LYS A	31	30.788	8.066	29.309	1.00	25.85	C
ATOM	156	CD	LYS A	31	31.154	7.355	30.605	1.00	29.83	C
ATOM	157	CE	LYS A	31	31.652	8.305	31.675	1.00	32.89	C
ATOM	158	NZ	LYS A	31	32.116	7.506	32.799	1.00	39.63	C
ATOM	159	N	TYR A	32	30.845	6.219	25.034	1.00	24.83	C
ATOM	160	CA	TYR A	32	30.565	5.424	23.844	1.00	22.31	O
ATOM	161	C	TYR A	32	31.607	4.359	23.767	1.00	19.55	C
ATOM	162	O	TYR A	32	32.759	4.667	23.946	1.00	22.18	C
ATOM	163	CB	TYR A	32	30.569	6.367	22.640	1.00	25.12	C
ATOM	164	CG	TYR A	32	30.557	5.725	21.262	1.00	27.46	C
ATOM	165	CD1	TYR A	32	31.790	5.449	20.689	1.00	26.41	C
ATOM	166	CD2	TYR A	32	29.369	5.437	20.613	1.00	26.10	O
ATOM	167	CE1	TYR A	32	31.871	4.860	19.452	1.00	27.56	N
ATOM	168	CE2	TYR A	32	29.462	4.854	19.356	1.00	29.60	C
ATOM	169	CZ	TYR A	32	30.710	4.589	18.787	1.00	28.41	C
ATOM	170	OH	TYR A	32	30.844	4.087	17.501	1.00	32.61	C
ATOM	171	N	VAL A	33	31.217	3.108	23.604	1.00	20.21	C
ATOM	172	CA	VAL A	33	32.138	2.022	23.453	1.00	22.23	C
ATOM	173	C	VAL A	33	32.829	2.212	22.110	1.00	24.20	C
ATOM	174	O	VAL A	33	32.156	2.231	21.078	1.00	24.76	O
ATOM	175	CB	VAL A	33	31.400	0.676	23.549	1.00	23.11	C
ATOM	176	CG1	VAL A	33	32.297	-0.537	23.309	1.00	22.36	C
ATOM	177	CG2	VAL A	33	30.857	0.535	24.951	1.00	25.26	N
ATOM	178	N	PRO A	34	34.158	2.380	22.078	1.00	25.19	C
ATOM	179	CA	PRO A	34	34.921	2.477	20.834	1.00	27.43	C
ATOM	180	C	PRO A	34	34.727	1.263	19.907	1.00	27.77	O
ATOM	181	O	PRO A	34	34.907	0.101	20.291	1.00	27.65	C
ATOM	182	CB	PRO A	34	36.381	2.586	21.335	1.00	29.54	C
ATOM	183	CG	PRO A	34	36.224	3.056	22.773	1.00	26.93	C
ATOM	184	CD	PRO A	34	35.043	2.269	23.245	1.00	23.54	C

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FIGURE 8A-14

ATOM	185	N	GLY	A	35	34.312	1.550	18.666	1.00	28.92	N
ATOM	186	CA	GLY	A	35	34.175	0.517	17.650	1.00	28.59	C
ATOM	187	C	GLY	A	35	32.886	-0.277	17.715	1.00	28.76	C
ATOM	188	O	GLY	A	35	32.743	-1.224	16.957	1.00	29.41	O
HETATM	189	N	MSE	A	36	31.923	0.064	18.569	1.00	27.95	N
HETATM	190	CA	MSE	A	36	30.612	-0.561	18.587	1.00	28.65	C
HETATM	191	C	MSE	A	36	29.809	-0.477	17.276	1.00	28.45	C
HETATM	192	O	MSE	A	36	28.824	-1.189	17.098	1.00	26.26	O
HETATM	193	CB	MSE	A	36	29.774	0.036	19.739	1.00	32.71	C
HETATM	194	CG	MSE	A	36	29.232	1.427	19.485	1.00	34.05	C
HETATM	195	SE	MSE	A	36	27.946	2.252	20.676	1.00	36.59	SE
HETATM	196	CE	MSE	A	36	26.309	1.728	19.841	1.00	26.94	C
ATOM	197	N	ASP	A	37	30.212	0.393	16.338	1.00	30.42	N
ATOM	198	CA	ASP	A	37	29.736	0.418	14.935	1.00	30.74	C
ATOM	199	C	ASP	A	37	30.051	-0.794	14.038	1.00	27.32	C
ATOM	200	O	ASP	A	37	29.344	-1.054	13.064	1.00	28.97	O
ATOM	201	CB	ASP	A	37	30.200	1.716	14.234	1.00	33.15	C
ATOM	202	CG	ASP	A	37	31.706	1.960	14.294	1.00	35.22	C
ATOM	203	OD1	ASP	A	37	32.230	2.247	15.374	1.00	42.04	O
ATOM	204	OD2	ASP	A	37	32.369	1.875	13.275	1.00	34.84	O
ATOM	205	N	VAL	A	38	31.054	-1.584	14.381	1.00	23.11	N
ATOM	206	CA	VAL	A	38	31.471	-2.713	13.566	1.00	23.69	C
ATOM	207	C	VAL	A	38	31.568	-4.045	14.389	1.00	26.12	C
ATOM	208	O	VAL	A	38	31.649	-5.172	13.882	1.00	27.25	O
ATOM	209	CB	VAL	A	38	32.741	-2.089	12.936	1.00	19.85	C
ATOM	210	CG1	VAL	A	38	34.023	-2.366	13.647	1.00	16.55	C
ATOM	211	CG2	VAL	A	38	32.825	-2.379	11.512	1.00	19.54	C
ATOM	212	N	LEU	A	39	31.464	-3.968	15.728	1.00	26.26	N
ATOM	213	CA	LEU	A	39	31.505	-5.113	16.640	1.00	26.07	C
ATOM	214	C	LEU	A	39	30.149	-5.788	16.888	1.00	25.48	C
ATOM	215	O	LEU	A	39	29.130	-5.109	16.842	1.00	23.47	O
ATOM	216	CB	LEU	A	39	32.061	-4.671	18.014	1.00	25.49	C
ATOM	217	CG	LEU	A	39	33.515	-4.307	18.156	1.00	27.97	C
ATOM	218	CD1	LEU	A	39	33.729	-3.645	19.510	1.00	30.79	C
ATOM	219	CD2	LEU	A	39	34.399	-5.522	17.940	1.00	23.69	C
ATOM	220	N	PRO	A	40	30.017	-7.086	17.192	1.00	25.65	N
ATOM	221	CA	PRO	A	40	28.734	-7.665	17.563	1.00	27.77	C
ATOM	222	C	PRO	A	40	28.061	-7.004	18.792	1.00	27.59	C
ATOM	223	O	PRO	A	40	28.710	-6.411	19.658	1.00	26.55	O
ATOM	224	CB	PRO	A	40	29.102	-9.122	17.683	1.00	27.41	C
ATOM	225	CG	PRO	A	40	30.584	-9.150	18.015	1.00	26.93	C
ATOM	226	CD	PRO	A	40	31.076	-8.082	17.099	1.00	26.35	C
ATOM	227	N	SER	A	41	26.724	-7.026	18.830	1.00	27.40	N
ATOM	228	CA	SER	A	41	26.003	-6.235	19.806	1.00	26.79	C
ATOM	229	C	SER	A	41	26.288	-6.707	21.202	1.00	27.70	C
ATOM	230	O	SER	A	41	26.451	-5.903	22.097	1.00	29.20	O
ATOM	231	CB	SER	A	41	24.540	-6.240	19.558	1.00	23.46	C
ATOM	232	OG	SER	A	41	24.074	-7.559	19.691	1.00	25.42	O
ATOM	233	N	HIS	A	42	26.526	-8.007	21.355	1.00	29.95	N
ATOM	234	CA	HIS	A	42	26.853	-8.594	22.636	1.00	30.32	C
ATOM	235	C	HIS	A	42	28.076	-7.971	23.312	1.00	29.42	C
ATOM	236	O	HIS	A	42	28.270	-8.138	24.524	1.00	28.56	O
ATOM	237	CB	HIS	A	42	27.008	-10.109	22.451	1.00	35.10	C
ATOM	238	CG	HIS	A	42	28.387	-10.616	21.997	1.00	39.36	C
ATOM	239	ND1	HIS	A	42	29.424	-10.993	22.752	1.00	43.05	N
ATOM	240	CD2	HIS	A	42	28.829	-10.644	20.694	1.00	42.30	C
ATOM	241	CE1	HIS	A	42	30.472	-11.198	21.971	1.00	42.05	C
ATOM	242	NE2	HIS	A	42	30.103	-10.969	20.735	1.00	41.31	N
ATOM	243	N	CYS	A	43	28.888	-7.246	22.533	1.00	26.69	C
ATOM	244	CA	CYS	A	43	30.112	-6.657	23.037	1.00	29.55	C

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FIGURE 8A-15

ATOM	245	C	CYS	A	43	29.916	-5.341	23.766	1.00	29.31	C
ATOM	246	O	CYS	A	43	30.779	-4.912	24.512	1.00	31.36	O
ATOM	247	CB	CYS	A	43	31.140	-6.395	21.915	1.00	31.15	C
ATOM	248	SG	CYS	A	43	31.674	-7.929	21.120	1.00	35.60	S
ATOM	249	N	TRP	A	44	28.813	-4.637	23.555	1.00	28.24	N
ATOM	250	CA	TRP	A	44	28.704	-3.240	23.952	1.00	25.54	C
ATOM	251	C	TRP	A	44	27.331	-2.947	24.498	1.00	25.35	C
ATOM	252	O	TRP	A	44	27.173	-1.924	25.113	1.00	28.50	O
ATOM	253	CB	TRP	A	44	28.965	-2.299	22.746	1.00	22.52	C
ATOM	254	CG	TRP	A	44	28.207	-2.626	21.450	1.00	20.09	C
ATOM	255	CD1	TRP	A	44	28.851	-3.316	20.455	1.00	19.03	C
ATOM	256	CD2	TRP	A	44	26.890	-2.326	21.142	1.00	20.02	C
ATOM	257	NE1	TRP	A	44	27.948	-3.464	19.527	1.00	20.48	N
ATOM	258	CE2	TRP	A	44	26.791	-2.877	19.882	1.00	19.41	C
ATOM	259	CE3	TRP	A	44	25.841	-1.609	21.652	1.00	18.83	C
ATOM	260	CZ2	TRP	A	44	25.665	-2.678	19.127	1.00	16.33	C
ATOM	261	CZ3	TRP	A	44	24.711	-1.431	20.910	1.00	16.81	C
ATOM	262	CH2	TRP	A	44	24.617	-1.962	19.653	1.00	17.88	C
ATOM	263	N	ILE	A	45	26.328	-3.786	24.275	1.00	27.39	N
ATOM	264	CA	ILE	A	45	24.934	-3.500	24.540	1.00	28.48	C
ATOM	265	C	ILE	A	45	24.666	-3.370	26.025	1.00	29.97	C
ATOM	266	O	ILE	A	45	23.770	-2.622	26.389	1.00	31.30	O
ATOM	267	CB	ILE	A	45	24.055	-4.601	23.904	1.00	28.39	C
ATOM	268	CG1	ILE	A	45	22.603	-4.220	23.795	1.00	28.24	C
ATOM	269	CG2	ILE	A	45	24.152	-5.926	24.668	1.00	28.54	C
ATOM	270	CD1	ILE	A	45	22.371	-2.868	23.098	1.00	30.38	C
ATOM	271	N	SER	A	46	25.408	-4.044	26.900	1.00	30.95	N
ATOM	272	CA	SER	A	46	25.200	-3.897	28.337	1.00	32.47	C
ATOM	273	C	SER	A	46	25.677	-2.546	28.844	1.00	30.61	C
ATOM	274	O	SER	A	46	24.974	-1.880	29.597	1.00	30.88	O
ATOM	275	CB	SER	A	46	25.899	-5.016	29.106	1.00	35.61	C
ATOM	276	OG	SER	A	46	25.387	-6.311	28.746	1.00	43.59	O
ATOM	277	N	GLU	A	47	26.840	-2.123	28.370	1.00	28.57	N
ATOM	278	CA	GLU	A	47	27.355	-0.823	28.680	1.00	28.90	C
ATOM	279	C	GLU	A	47	26.567	0.306	28.090	1.00	27.44	C
ATOM	280	O	GLU	A	47	26.383	1.323	28.735	1.00	28.17	O
ATOM	281	CB	GLU	A	47	28.791	-0.702	28.244	1.00	30.74	C
ATOM	282	CG	GLU	A	47	29.439	0.554	28.818	1.00	34.60	C
ATOM	283	CD	GLU	A	47	29.550	0.665	30.351	1.00	37.52	C
ATOM	284	OE1	GLU	A	47	28.998	-0.153	31.107	1.00	37.54	O
ATOM	285	OE2	GLU	A	47	30.208	1.607	30.800	1.00	38.33	O
HETATM	286	N	MSE	A	48	26.073	0.098	26.879	1.00	27.89	N
HETATM	287	CA	MSE	A	48	25.327	1.113	26.154	1.00	28.18	C
HETATM	288	C	MSE	A	48	23.945	1.421	26.667	1.00	26.21	C
HETATM	289	O	MSE	A	48	23.580	2.578	26.606	1.00	27.02	O
HETATM	290	CB	MSE	A	48	25.309	0.882	24.637	1.00	29.23	C
HETATM	291	CG	MSE	A	48	26.739	1.048	24.095	1.00	28.12	C
HETATM	292	SE	MSE	A	48	27.685	2.655	24.690	1.00	35.61	SE
HETATM	293	CE	MSE	A	48	26.476	3.857	23.743	1.00	22.58	C
ATOM	294	N	VAL	A	49	23.147	0.491	27.195	1.00	27.65	N
ATOM	295	CA	VAL	A	49	21.882	0.875	27.814	1.00	27.43	C
ATOM	296	C	VAL	A	49	22.017	1.680	29.115	1.00	27.42	C
ATOM	297	O	VAL	A	49	21.224	2.595	29.394	1.00	27.48	O
ATOM	298	CB	VAL	A	49	20.884	-0.284	27.907	1.00	27.18	C
ATOM	299	CG1	VAL	A	49	20.438	-0.478	26.452	1.00	27.08	C
ATOM	300	CG2	VAL	A	49	21.421	-1.534	28.610	1.00	23.66	C
ATOM	301	N	VAL	A	50	23.100	1.370	29.847	1.00	26.26	N
ATOM	302	CA	VAL	A	50	23.469	2.060	31.068	1.00	24.75	C
ATOM	303	C	VAL	A	50	23.964	3.431	30.716	1.00	25.57	C
ATOM	304	O	VAL	A	50	23.485	4.384	31.320	1.00	28.77	O

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FIGURE 8A-16

ATOM	305	CB	VAL	A	50	24.545	1.307	31.812	1.00	24.44	
ATOM	306	CG1	VAL	A	50	25.062	2.106	32.969	1.00	23.79	C
ATOM	307	CG2	VAL	A	50	23.952	0.040	32.382	1.00	24.17	C
ATOM	308	N	GLN	A	51	24.888	3.551	29.758	1.00	22.88	N
ATOM	309	CA	GLN	A	51	25.315	4.841	29.294	1.00	18.59	C
ATOM	310	C	GLN	A	51	24.226	5.698	28.700	1.00	18.17	O
ATOM	311	O	GLN	A	51	24.223	6.904	28.948	1.00	20.05	C
ATOM	312	CB	GLN	A	51	26.474	4.707	28.320	1.00	21.19	C
ATOM	313	CG	GLN	A	51	27.676	4.059	28.934	1.00	17.37	C
ATOM	314	CD	GLN	A	51	28.072	4.720	30.240	1.00	21.56	O
ATOM	315	OE1	GLN	A	51	27.879	5.913	30.476	1.00	23.67	N
ATOM	316	NE2	GLN	A	51	28.662	3.969	31.152	1.00	22.77	N
ATOM	317	N	LEU	A	52	23.291	5.106	27.959	1.00	15.38	C
ATOM	318	CA	LEU	A	52	22.210	5.850	27.374	1.00	16.72	O
ATOM	319	C	LEU	A	52	21.199	6.284	28.411	1.00	18.34	C
ATOM	320	O	LEU	A	52	20.676	7.387	28.382	1.00	18.73	C
ATOM	321	CB	LEU	A	52	21.533	5.006	26.309	1.00	15.91	C
ATOM	322	CG	LEU	A	52	22.207	5.059	24.928	1.00	17.11	C
ATOM	323	CD1	LEU	A	52	21.807	3.849	24.155	1.00	14.42	N
ATOM	324	CD2	LEU	A	52	21.886	6.330	24.184	1.00	12.26	C
ATOM	325	N	SER	A	53	20.932	5.433	29.378	1.00	20.83	C
ATOM	326	CA	SER	A	53	20.098	5.806	30.505	1.00	23.79	O
ATOM	327	C	SER	A	53	20.716	6.966	31.295	1.00	24.20	C
ATOM	328	O	SER	A	53	19.977	7.897	31.624	1.00	26.42	O
ATOM	329	CB	SER	A	53	19.917	4.605	31.403	1.00	23.71	O
ATOM	330	OG	SER	A	53	19.285	5.024	32.601	1.00	30.23	N
ATOM	331	N	ASP	A	54	22.043	6.977	31.559	1.00	23.25	C
ATOM	332	CA	ASP	A	54	22.687	8.036	32.308	1.00	20.61	C
ATOM	333	C	ASP	A	54	22.659	9.325	31.572	1.00	19.02	O
ATOM	334	O	ASP	A	54	22.303	10.358	32.142	1.00	20.41	C
ATOM	335	CB	ASP	A	54	24.114	7.682	32.740	1.00	25.54	C
ATOM	336	CG	ASP	A	54	24.207	6.579	33.815	1.00	31.33	O
ATOM	337	OD1	ASP	A	54	23.185	5.965	34.178	1.00	36.02	O
ATOM	338	OD2	ASP	A	54	25.318	6.318	34.307	1.00	32.62	N
ATOM	339	N	SER	A	55	22.962	9.286	30.291	1.00	16.79	C
ATOM	340	CA	SER	A	55	22.857	10.514	29.541	1.00	17.42	C
ATOM	341	C	SER	A	55	21.454	11.096	29.425	1.00	16.81	O
ATOM	342	O	SER	A	55	21.293	12.318	29.474	1.00	17.95	C
ATOM	343	CB	SER	A	55	23.511	10.378	28.150	1.00	18.91	O
ATOM	344	OG	SER	A	55	24.863	9.936	28.237	1.00	22.06	N
ATOM	345	N	LEU	A	56	20.439	10.249	29.243	1.00	17.01	C
ATOM	346	CA	LEU	A	56	19.073	10.726	29.162	1.00	17.99	C
ATOM	347	C	LEU	A	56	18.518	11.188	30.514	1.00	18.27	O
ATOM	348	O	LEU	A	56	17.800	12.186	30.575	1.00	18.82	C
ATOM	349	CB	LEU	A	56	18.130	9.712	28.505	1.00	17.68	C
ATOM	350	CG	LEU	A	56	18.061	9.584	26.983	1.00	18.44	C
ATOM	351	CD1	LEU	A	56	17.381	8.280	26.613	1.00	19.03	N
ATOM	352	CD2	LEU	A	56	17.392	10.764	26.321	1.00	16.39	C
ATOM	353	N	THR	A	57	18.835	10.532	31.616	1.00	18.45	O
ATOM	354	CA	THR	A	57	18.376	11.005	32.911	1.00	21.42	C
ATOM	355	C	THR	A	57	18.975	12.383	33.205	1.00	21.42	C
ATOM	356	O	THR	A	57	18.263	13.287	33.640	1.00	21.53	O
ATOM	357	CB	THR	A	57	18.680	9.942	33.948	1.00	18.39	C
ATOM	358	OG1	THR	A	57	18.055	8.791	33.418	1.00	20.01	O
ATOM	359	CG2	THR	A	57	17.980	10.190	35.253	1.00	23.58	O
ATOM	360	N	ASP	A	58	20.245	12.587	32.819	1.00	23.66	N
ATOM	361	CA	ASP	A	58	20.908	13.867	32.971	1.00	24.99	C
ATOM	362	C	ASP	A	58	20.269	14.969	32.162	1.00	23.11	C
ATOM	363	O	ASP	A	58	20.243	16.133	32.567	1.00	22.89	O
ATOM	364	CB	ASP	A	58	22.410	13.766	32.646	1.00	33.60	C

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FIGURE 8A-17

ATOM	365	CG	ASP	A	58	23.101	15.151	32.595	1.00	41.66
ATOM	366	OD1	ASP	A	58	23.500	15.636	33.666	1.00	45.37
ATOM	367	OD2	ASP	A	58	23.204	15.764	31.502	1.00	43.30
ATOM	368	N	LEU	A	59	19.762	14.614	30.994	1.00	21.38
ATOM	369	CA	LEU	A	59	19.106	15.568	30.124	1.00	19.63
ATOM	370	C	LEU	A	59	17.857	16.179	30.719	1.00	20.35
ATOM	371	O	LEU	A	59	17.522	17.321	30.413	1.00	19.57
ATOM	372	CB	LEU	A	59	18.751	14.826	28.859	1.00	19.31
ATOM	373	CG	LEU	A	59	19.006	15.498	27.551	1.00	18.41
ATOM	374	CD1	LEU	A	59	20.161	16.496	27.615	1.00	16.32
ATOM	375	CD2	LEU	A	59	19.225	14.401	26.555	1.00	17.59
ATOM	376	N	LEU	A	60	17.163	15.410	31.587	1.00	21.63
ATOM	377	CA	LEU	A	60	15.930	15.857	32.216	1.00	20.55
ATOM	378	C	LEU	A	60	16.133	17.147	32.974	1.00	22.32
ATOM	379	O	LEU	A	60	15.264	18.016	32.929	1.00	23.28
ATOM	380	CB	LEU	A	60	15.389	14.796	33.145	1.00	17.67
ATOM	381	CG	LEU	A	60	14.680	13.601	32.538	1.00	14.57
ATOM	382	CD1	LEU	A	60	14.293	12.641	33.643	1.00	12.83
ATOM	383	CD2	LEU	A	60	13.462	14.048	31.847	1.00	8.22
ATOM	384	N	ASP	A	61	17.338	17.285	33.558	1.00	22.42
ATOM	385	CA	ASP	A	61	17.805	18.483	34.247	1.00	22.10
ATOM	386	C	ASP	A	61	17.810	19.768	33.433	1.00	20.08
ATOM	387	O	ASP	A	61	17.841	20.870	33.974	1.00	20.02
ATOM	388	CB	ASP	A	61	19.203	18.169	34.753	1.00	28.60
ATOM	389	CG	ASP	A	61	19.803	19.159	35.750	1.00	34.29
ATOM	390	OD1	ASP	A	61	19.459	19.073	36.931	1.00	40.97
ATOM	391	OD2	ASP	A	61	20.616	20.006	35.356	1.00	37.85
ATOM	392	N	LYS	A	62	17.721	19.693	32.105	1.00	19.76
ATOM	393	CA	LYS	A	62	17.839	20.862	31.245	1.00	16.53
ATOM	394	C	LYS	A	62	16.485	21.335	30.770	1.00	16.75
ATOM	395	O	LYS	A	62	16.388	22.383	30.130	1.00	17.62
ATOM	396	CB	LYS	A	62	18.684	20.529	30.020	1.00	18.65
ATOM	397	CG	LYS	A	62	19.986	19.755	30.233	1.00	16.80
ATOM	398	CD	LYS	A	62	20.808	20.483	31.276	1.00	18.07
ATOM	399	CE	LYS	A	62	22.135	19.776	31.535	1.00	23.34
ATOM	400	NZ	LYS	A	62	22.088	18.331	31.330	1.00	28.06
ATOM	401	N	PHE	A	63	15.400	20.605	31.068	1.00	16.40
ATOM	402	CA	PHE	A	63	14.086	20.979	30.586	1.00	16.93
ATOM	403	C	PHE	A	63	13.110	21.140	31.730	1.00	17.40
ATOM	404	O	PHE	A	63	13.294	20.626	32.826	1.00	17.50
ATOM	405	CB	PHE	A	63	13.576	19.942	29.574	1.00	15.08
ATOM	406	CG	PHE	A	63	14.424	19.850	28.325	1.00	13.39
ATOM	407	CD1	PHE	A	63	14.261	20.767	27.317	1.00	13.60
ATOM	408	CD2	PHE	A	63	15.410	18.888	28.252	1.00	14.95
ATOM	409	CE1	PHE	A	63	15.126	20.740	26.266	1.00	10.99
ATOM	410	CE2	PHE	A	63	16.305	18.889	27.207	1.00	14.45
ATOM	411	CZ	PHE	A	63	16.150	19.832	26.229	1.00	10.95
ATOM	412	N	SER	A	64	12.031	21.843	31.444	1.00	19.14
ATOM	413	CA	SER	A	64	10.993	22.080	32.407	1.00	21.71
ATOM	414	C	SER	A	64	9.832	21.125	32.198	1.00	22.87
ATOM	415	O	SER	A	64	9.431	20.758	31.098	1.00	24.09
ATOM	416	CB	SER	A	64	10.533	23.508	32.261	1.00	22.47
ATOM	417	OG	SER	A	64	9.408	23.881	33.049	1.00	29.46
ATOM	418	N	ASN	A	65	9.298	20.809	33.363	1.00	23.97
ATOM	419	CA	ASN	A	65	8.233	19.855	33.608	1.00	29.13
ATOM	420	C	ASN	A	65	6.899	20.530	33.390	1.00	31.34
ATOM	421	O	ASN	A	65	5.883	19.858	33.203	1.00	35.27
ATOM	422	CB	ASN	A	65	8.309	19.551	35.119	1.00	30.43
ATOM	423	CG	ASN	A	65	8.097	18.117	35.514	1.00	33.16
ATOM	424	OD1	ASN	A	65	7.488	17.258	34.873	1.00	41.60

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FIGURE 8A-18

ATOM	425	ND2	ASN	A	65	8.641	17.823	36.656	1.00	34.77
ATOM	426	N	ILE	A	66	6.892	21.862	33.561	1.00	32.62
ATOM	427	CA	ILE	A	66	5.708	22.691	33.384	1.00	33.83
ATOM	428	C	ILE	A	66	5.681	23.071	31.918	1.00	35.58
ATOM	429	O	ILE	A	66	6.450	23.910	31.431	1.00	36.08
ATOM	430	CB	ILE	A	66	5.752	24.000	34.223	1.00	33.21
ATOM	431	CG1	ILE	A	66	6.162	23.831	35.672	1.00	33.50
ATOM	432	CG2	ILE	A	66	4.416	24.708	34.158	1.00	31.21
ATOM	433	CD1	ILE	A	66	5.330	22.784	36.415	1.00	32.37
ATOM	434	N	SER	A	67	4.782	22.424	31.201	1.00	37.23
ATOM	435	CA	SER	A	67	4.669	22.650	29.771	1.00	40.50
ATOM	436	C	SER	A	67	3.358	22.008	29.327	1.00	42.07
ATOM	437	O	SER	A	67	3.073	20.841	29.622	1.00	43.86
ATOM	438	CB	SER	A	67	5.892	21.985	29.075	1.00	40.62
ATOM	439	OG	SER	A	67	6.244	22.539	27.815	1.00	36.76
ATOM	440	N	GLU	A	68	2.502	22.765	28.648	1.00	44.40
ATOM	441	CA	GLU	A	68	1.317	22.183	28.023	1.00	46.43
ATOM	442	C	GLU	A	68	1.777	21.448	26.758	1.00	46.20
ATOM	443	O	GLU	A	68	2.874	21.690	26.234	1.00	47.39
ATOM	444	CB	GLU	A	68	0.364	23.301	27.637	1.00	49.01
ATOM	445	CG	GLU	A	68	-1.051	22.858	27.256	1.00	53.42
ATOM	446	CD	GLU	A	68	-2.066	23.229	28.324	1.00	56.12
ATOM	447	OE1	GLU	A	68	-2.255	22.391	29.223	1.00	58.37
ATOM	448	OE2	GLU	A	68	-2.634	24.342	28.250	1.00	56.09
ATOM	449	N	GLY	A	69	0.957	20.523	26.262	1.00	45.44
ATOM	450	CA	GLY	A	69	1.228	19.834	25.021	1.00	43.62
ATOM	451	C	GLY	A	69	2.561	19.130	25.029	1.00	42.33
ATOM	452	O	GLY	A	69	2.944	18.429	25.963	1.00	43.42
ATOM	453	N	LEU	A	70	3.245	19.412	23.927	1.00	42.01
ATOM	454	CA	LEU	A	70	4.567	18.856	23.634	1.00	40.66
ATOM	455	C	LEU	A	70	5.570	19.283	24.688	1.00	37.48
ATOM	456	O	LEU	A	70	5.769	20.477	24.916	1.00	39.56
ATOM	457	CB	LEU	A	70	5.069	19.339	22.221	1.00	42.73
ATOM	458	CG	LEU	A	70	6.365	18.753	21.553	1.00	43.68
ATOM	459	CD1	LEU	A	70	6.429	17.212	21.539	1.00	40.99
ATOM	460	CD2	LEU	A	70	6.506	19.318	20.134	1.00	42.81
ATOM	461	N	SER	A	71	6.203	18.289	25.301	1.00	32.14
ATOM	462	CA	SER	A	71	7.187	18.514	26.330	1.00	24.30
ATOM	463	C	SER	A	71	8.394	17.653	26.032	1.00	20.06
ATOM	464	O	SER	A	71	8.282	16.449	25.900	1.00	21.51
ATOM	465	CB	SER	A	71	6.519	18.160	27.653	1.00	21.80
ATOM	466	OG	SER	A	71	7.393	18.171	28.756	1.00	17.14
ATOM	467	N	ASN	A	72	9.573	18.208	25.883	1.00	18.83
ATOM	468	CA	ASN	A	72	10.787	17.419	25.827	1.00	16.99
ATOM	469	C	ASN	A	72	11.079	16.692	27.083	1.00	15.54
ATOM	470	O	ASN	A	72	11.566	15.578	26.997	1.00	16.64
ATOM	471	CB	ASN	A	72	11.982	18.277	25.558	1.00	20.15
ATOM	472	CG	ASN	A	72	11.916	18.839	24.158	1.00	23.44
ATOM	473	OD1	ASN	A	72	11.109	18.421	23.317	1.00	25.67
ATOM	474	ND2	ASN	A	72	12.780	19.812	23.894	1.00	24.59
ATOM	475	N	TYR	A	73	10.823	17.309	28.239	1.00	15.06
ATOM	476	CA	TYR	A	73	10.835	16.579	29.507	1.00	15.26
ATOM	477	C	TYR	A	73	9.986	15.319	29.443	1.00	15.85
ATOM	478	O	TYR	A	73	10.538	14.262	29.740	1.00	18.32
ATOM	479	CB	TYR	A	73	10.315	17.410	30.733	1.00	12.75
ATOM	480	CG	TYR	A	73	10.760	16.862	32.082	1.00	10.27
ATOM	481	CD1	TYR	A	73	11.940	17.306	32.624	1.00	11.84
ATOM	482	CD2	TYR	A	73	9.993	15.928	32.769	1.00	14.03
ATOM	483	CE1	TYR	A	73	12.364	16.827	33.839	1.00	12.67
ATOM	484	CE2	TYR	A	73	10.412	15.419	33.979	1.00	10.24

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FIGURE 8A-19

ATOM	485	CZ	TYR	A	73	11.592	15.891	34.491	1.00 14.02
ATOM	486	OH	TYR	A	73	12.042	15.429	35.703	1.00 14.54
ATOM	487	N	SER	A	74	8.682	15.323	29.087	1.00 18.48
ATOM	488	CA	SER	A	74	7.947	14.076	29.034	1.00 18.74
ATOM	489	C	SER	A	74	8.429	13.074	28.017	1.00 18.80
ATOM	490	O	SER	A	74	8.430	11.882	28.327	1.00 18.69
ATOM	491	CB	SER	A	74	6.434	14.228	29.002	1.00 21.96
ATOM	492	OG	SER	A	74	5.847	15.278	28.253	1.00 30.65
ATOM	493	N	ILE	A	75	8.928	13.522	26.849	1.00 18.95
ATOM	494	CA	ILE	A	75	9.481	12.602	25.855	1.00 17.82
ATOM	495	C	ILE	A	75	10.689	11.896	26.422	1.00 17.12
ATOM	496	O	ILE	A	75	10.679	10.688	26.557	1.00 18.03
ATOM	497	CB	ILE	A	75	9.750	13.298	24.460	1.00 20.42
ATOM	498	CG1	ILE	A	75	8.440	13.885	23.860	1.00 19.63
ATOM	499	CG2	ILE	A	75	10.327	12.283	23.471	1.00 17.30
ATOM	500	CD1	ILE	A	75	8.582	14.604	22.508	1.00 23.08
ATOM	501	N	ILE	A	76	11.698	12.625	26.857	1.00 18.46
ATOM	502	CA	ILE	A	76	12.916	12.070	27.436	1.00 19.33
ATOM	503	C	ILE	A	76	12.622	11.116	28.592	1.00 19.01
ATOM	504	O	ILE	A	76	13.199	10.040	28.714	1.00 20.65
ATOM	505	CB	ILE	A	76	13.816	13.253	27.900	1.00 18.88
ATOM	506	CG1	ILE	A	76	14.239	14.216	26.789	1.00 17.98
ATOM	507	CG2	ILE	A	76	15.057	12.732	28.600	1.00 20.53
ATOM	508	CD1	ILE	A	76	14.950	15.500	27.300	1.00 15.54
ATOM	509	N	ASP	A	77	11.643	11.474	29.412	1.00 19.90
ATOM	510	CA	ASP	A	77	11.226	10.682	30.562	1.00 19.93
ATOM	511	C	ASP	A	77	10.627	9.341	30.177	1.00 21.32
ATOM	512	O	ASP	A	77	10.832	8.318	30.830	1.00 21.41
ATOM	513	CB	ASP	A	77	10.189	11.524	31.263	1.00 21.00
ATOM	514	CG	ASP	A	77	9.506	10.808	32.390	1.00 23.32
ATOM	515	OD1	ASP	A	77	10.211	10.249	33.204	1.00 26.02
ATOM	516	OD2	ASP	A	77	8.283	10.750	32.419	1.00 24.74
ATOM	517	N	LYS	A	78	9.835	9.312	29.101	1.00 23.41
ATOM	518	CA	LYS	A	78	9.385	8.038	28.606	1.00 23.09
ATOM	519	C	LYS	A	78	10.529	7.247	27.975	1.00 24.61
ATOM	520	O	LYS	A	78	10.518	6.000	28.021	1.00 26.85
ATOM	521	CB	LYS	A	78	8.267	8.237	27.656	1.00 25.84
ATOM	522	CG	LYS	A	78	7.024	8.643	28.403	1.00 29.26
ATOM	523	CD	LYS	A	78	5.882	8.766	27.362	1.00 40.97
ATOM	524	CE	LYS	A	78	6.119	9.815	26.221	1.00 43.91
ATOM	525	NZ	LYS	A	78	5.056	9.792	25.229	1.00 48.24
ATOM	526	N	LEU	A	79	11.559	7.936	27.437	1.00 22.19
ATOM	527	CA	LEU	A	79	12.718	7.253	26.865	1.00 18.09
ATOM	528	C	LEU	A	79	13.577	6.757	27.968	1.00 16.82
ATOM	529	O	LEU	A	79	14.146	5.692	27.806	1.00 17.74
ATOM	530	CB	LEU	A	79	13.580	8.147	25.986	1.00 16.97
ATOM	531	CG	LEU	A	79	12.928	8.748	24.768	1.00 15.98
ATOM	532	CD1	LEU	A	79	13.984	9.540	24.058	1.00 16.93
ATOM	533	CD2	LEU	A	79	12.264	7.721	23.857	1.00 14.76
ATOM	534	N	VAL	A	80	13.609	7.460	29.101	1.00 16.48
ATOM	535	CA	VAL	A	80	14.352	6.994	30.249	1.00 13.79
ATOM	536	C	VAL	A	80	13.697	5.725	30.731	1.00 14.44
ATOM	537	O	VAL	A	80	14.385	4.763	31.022	1.00 14.81
ATOM	538	CB	VAL	A	80	14.382	8.054	31.331	1.00 17.12
ATOM	539	CG1	VAL	A	80	14.937	7.490	32.631	1.00 17.65
ATOM	540	CG2	VAL	A	80	15.307	9.189	30.910	1.00 13.43
ATOM	541	N	ASN	A	81	12.383	5.633	30.743	1.00 16.27
ATOM	542	CA	ASN	A	81	11.696	4.398	31.081	1.00 18.71
ATOM	543	C	ASN	A	81	11.852	3.174	30.176	1.00 21.49
ATOM	544	O	ASN	A	81	11.945	2.060	30.691	1.00 22.57

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FIGURE 8A-20

ATOM	545	CB	ASN	A	81	10.244	4.707	31.191	1.00	20.64	C
ATOM	546	CG	ASN	A	81	9.968	5.574	32.402	1.00	22.06	C
ATOM	547	OD1	ASN	A	81	10.652	5.475	33.422	1.00	22.22	O
ATOM	548	ND2	ASN	A	81	8.941	6.409	32.322	1.00	21.76	N
ATOM	549	N	ILE	A	82	11.898	3.339	28.846	1.00	21.86	N
ATOM	550	CA	ILE	A	82	12.226	2.270	27.917	1.00	23.02	C
ATOM	551	C	ILE	A	82	13.602	1.742	28.112	1.00	23.67	C
ATOM	552	O	ILE	A	82	13.728	0.536	28.067	1.00	26.85	O
ATOM	553	CB	ILE	A	82	12.089	2.768	26.497	1.00	22.79	C
ATOM	554	CG1	ILE	A	82	10.613	2.757	26.220	1.00	23.80	C
ATOM	555	CG2	ILE	A	82	12.854	1.951	25.474	1.00	21.98	C
ATOM	556	CD1	ILE	A	82	10.321	3.659	25.020	1.00	27.18	C
ATOM	557	N	VAL	A	83	14.619	2.586	28.254	1.00	25.82	N
ATOM	558	CA	VAL	A	83	15.996	2.104	28.338	1.00	27.82	C
ATOM	559	C	VAL	A	83	16.212	1.471	29.706	1.00	30.01	C
ATOM	560	O	VAL	A	83	16.995	0.522	29.796	1.00	32.08	O
ATOM	561	CB	VAL	A	83	17.139	3.137	28.252	1.00	26.25	C
ATOM	562	CG1	VAL	A	83	18.343	2.445	27.683	1.00	28.68	C
ATOM	563	CG2	VAL	A	83	16.883	4.437	27.569	1.00	28.99	C
ATOM	564	N	ASP	A	84	15.602	1.983	30.789	1.00	30.99	N
ATOM	565	CA	ASP	A	84	15.711	1.384	32.123	1.00	34.08	C
ATOM	566	C	ASP	A	84	15.125	-0.013	32.275	1.00	34.30	C
ATOM	567	O	ASP	A	84	15.666	-0.816	33.035	1.00	35.01	O
ATOM	568	CB	ASP	A	84	15.148	2.331	33.189	1.00	37.32	C
ATOM	569	CG	ASP	A	84	15.909	3.664	33.316	1.00	42.03	C
ATOM	570	OD1	ASP	A	84	16.907	3.865	32.621	1.00	43.39	O
ATOM	571	OD2	ASP	A	84	15.496	4.523	34.107	1.00	44.86	O
ATOM	572	N	ASP	A	85	14.055	-0.335	31.524	1.00	35.79	N
ATOM	573	CA	ASP	A	85	13.554	-1.707	31.332	1.00	37.15	C
ATOM	574	C	ASP	A	85	14.655	-2.665	30.860	1.00	34.71	C
ATOM	575	O	ASP	A	85	14.777	-3.800	31.308	1.00	33.69	O
ATOM	576	CB	ASP	A	85	12.434	-1.780	30.233	1.00	42.27	C
ATOM	577	CG	ASP	A	85	11.023	-1.216	30.474	1.00	46.16	C
ATOM	578	OD1	ASP	A	85	10.747	-0.756	31.587	1.00	46.14	O
ATOM	579	OD2	ASP	A	85	10.197	-1.234	29.539	1.00	50.79	O
ATOM	580	N	LEU	A	86	15.437	-2.164	29.904	1.00	33.83	N
ATOM	581	CA	LEU	A	86	16.527	-2.886	29.288	1.00	33.71	C
ATOM	582	C	LEU	A	86	17.747	-2.959	30.177	1.00	34.12	C
ATOM	583	O	LEU	A	86	18.440	-3.965	30.083	1.00	34.86	O
ATOM	584	CB	LEU	A	86	16.907	-2.260	27.948	1.00	31.87	C
ATOM	585	CG	LEU	A	86	15.878	-2.198	26.829	1.00	30.75	C
ATOM	586	CD1	LEU	A	86	16.383	-1.351	25.699	1.00	30.54	C
ATOM	587	CD2	LEU	A	86	15.521	-3.581	26.349	1.00	29.51	C
ATOM	588	N	VAL	A	87	18.033	-1.973	31.039	1.00	33.89	N
ATOM	589	CA	VAL	A	87	19.121	-2.074	32.009	1.00	35.56	C
ATOM	590	C	VAL	A	87	18.933	-3.223	33.039	1.00	40.73	O
ATOM	591	O	VAL	A	87	19.889	-3.890	33.493	1.00	42.23	C
ATOM	592	CB	VAL	A	87	19.239	-0.695	32.614	1.00	31.60	C
ATOM	593	CG1	VAL	A	87	20.272	-0.634	33.703	1.00	33.57	N
ATOM	594	CG2	VAL	A	87	19.680	0.253	31.537	1.00	29.91	C
ATOM	595	N	GLU	A	88	17.645	-3.484	33.340	1.00	44.00	O
ATOM	596	CA	GLU	A	88	17.191	-4.563	34.217	1.00	47.21	C
ATOM	597	C	GLU	A	88	17.016	-5.918	33.542	1.00	48.21	C
ATOM	598	O	GLU	A	88	17.359	-6.909	34.169	1.00	47.84	N
ATOM	599	CB	GLU	A	88	15.868	-4.200	34.886	1.00	49.05	C
ATOM	600	CG	GLU	A	88	15.877	-2.952	35.772	1.00	52.09	O
ATOM	601	CD	GLU	A	88	16.809	-3.020	36.976	1.00	53.70	C
ATOM	602	OE1	GLU	A	88	16.608	-3.858	37.861	1.00	55.01	C
ATOM	603	OE2	GLU	A	88	17.744	-2.221	37.020	1.00	54.23	O
ATOM	604	N	CYS	A	89	16.475	-6.018	32.311	1.00	50.79	N

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FIGURE 8A-21

ATOM	605	CA	CYS	A	89	16.489	-7.244	31.503	1.00	54.51	C
ATOM	606	C	CYS	A	89	17.952	-7.703	31.459	1.00	55.09	C
ATOM	607	O	CYS	A	89	18.231	-8.791	31.961	1.00	57.42	O
ATOM	608	CB	CYS	A	89	15.903	-6.972	30.078	1.00	57.17	C
ATOM	609	SG	CYS	A	89	15.060	-8.280	29.096	1.00	64.80	S
ATOM	610	N	VAL	A	90	18.890	-6.838	31.002	1.00	55.69	N
ATOM	611	CA	VAL	A	90	20.357	-7.027	31.060	1.00	55.91	C
ATOM	612	C	VAL	A	90	20.906	-7.397	32.450	1.00	57.84	C
ATOM	613	O	VAL	A	90	22.014	-7.924	32.546	1.00	58.27	O
ATOM	614	CB	VAL	A	90	21.074	-5.738	30.480	1.00	53.45	C
ATOM	615	CG1	VAL	A	90	22.542	-5.564	30.824	1.00	52.76	C
ATOM	616	CG2	VAL	A	90	20.965	-5.689	28.978	1.00	50.05	C
ATOM	617	N	LYS	A	91	20.212	-7.128	33.558	1.00	59.29	N
ATOM	618	CA	LYS	A	91	20.556	-7.785	34.810	1.00	62.11	C
ATOM	619	C	LYS	A	91	19.865	-9.163	34.996	1.00	63.85	C
ATOM	620	O	LYS	A	91	20.517	-10.061	35.533	1.00	66.48	O
ATOM	621	CB	LYS	A	91	20.305	-6.837	35.993	1.00	61.39	C
ATOM	622	N	SER	A	104	36.757	4.074	31.300	1.00	64.71	N
ATOM	623	CA	SER	A	104	36.147	4.043	29.974	1.00	64.00	C
ATOM	624	C	SER	A	104	34.723	3.416	29.904	1.00	61.57	C
ATOM	625	O	SER	A	104	34.321	2.749	30.871	1.00	62.78	O
ATOM	626	CB	SER	A	104	37.147	3.441	28.919	1.00	65.90	C
ATOM	627	OG	SER	A	104	38.150	4.399	28.533	1.00	67.30	O
ATOM	628	N	PRO	A	105	33.891	3.576	28.842	1.00	57.26	N
ATOM	629	CA	PRO	A	105	34.173	4.332	27.635	1.00	53.19	C
ATOM	630	C	PRO	A	105	34.452	5.801	27.827	1.00	51.76	C
ATOM	631	O	PRO	A	105	34.107	6.397	28.848	1.00	53.30	O
ATOM	632	CB	PRO	A	105	32.968	4.091	26.813	1.00	51.85	C
ATOM	633	CG	PRO	A	105	31.869	3.765	27.755	1.00	53.45	C
ATOM	634	CD	PRO	A	105	32.618	2.880	28.698	1.00	55.74	C
ATOM	635	N	GLU	A	106	35.242	6.296	26.875	1.00	50.80	N
ATOM	636	CA	GLU	A	106	35.584	7.700	26.790	1.00	47.97	C
ATOM	637	C	GLU	A	106	34.332	8.435	26.350	1.00	44.14	C
ATOM	638	O	GLU	A	106	33.684	8.006	25.400	1.00	42.91	O
ATOM	639	CB	GLU	A	106	36.796	7.970	25.858	1.00	51.71	C
ATOM	640	CG	GLU	A	106	36.873	7.196	24.509	1.00	57.13	C
ATOM	641	CD	GLU	A	106	38.045	6.192	24.389	1.00	60.78	C
ATOM	642	OE1	GLU	A	106	38.141	5.251	25.189	1.00	61.59	O
ATOM	643	OE2	GLU	A	106	38.874	6.338	23.482	1.00	63.52	O
ATOM	644	N	PRO	A	107	33.936	9.481	27.092	1.00	41.02	N
ATOM	645	CA	PRO	A	107	32.846	10.386	26.770	1.00	38.74	C
ATOM	646	C	PRO	A	107	33.069	11.190	25.517	1.00	37.93	C
ATOM	647	O	PRO	A	107	34.148	11.749	25.271	1.00	40.00	O
ATOM	648	CB	PRO	A	107	32.764	11.292	27.970	1.00	39.85	C
ATOM	649	CG	PRO	A	107	34.162	11.290	28.542	1.00	40.91	C
ATOM	650	CD	PRO	A	107	34.522	9.832	28.384	1.00	41.30	C
ATOM	651	N	ARG	A	108	32.000	11.208	24.724	1.00	35.40	N
ATOM	652	CA	ARG	A	108	32.006	11.864	23.436	1.00	33.34	C
ATOM	653	C	ARG	A	108	30.766	12.722	23.318	1.00	29.75	C
ATOM	654	O	ARG	A	108	29.727	12.347	23.867	1.00	29.55	O
ATOM	655	CB	ARG	A	108	32.102	10.859	22.297	1.00	35.14	C
ATOM	656	CG	ARG	A	108	33.480	10.219	22.313	1.00	39.55	C
ATOM	657	CD	ARG	A	108	33.734	9.386	21.057	1.00	44.05	C
ATOM	658	NE	ARG	A	108	34.715	8.324	21.284	1.00	45.36	N
ATOM	659	CZ	ARG	A	108	34.965	7.376	20.373	1.00	45.18	C
ATOM	660	NH1	ARG	A	108	34.481	7.446	19.142	1.00	46.89	N
ATOM	661	NH2	ARG	A	108	35.679	6.306	20.712	1.00	46.89	N
ATOM	662	N	LEU	A	109	30.932	13.877	22.650	1.00	26.42	N
ATOM	663	CA	LEU	A	109	29.833	14.770	22.334	1.00	25.17	C
ATOM	664	C	LEU	A	109	29.126	14.453	21.020	1.00	25.96	C

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FIGURE 8A-22

ATOM	665	O	LEU	A	109	29.774	14.229	20.002	1.00	26.43	O
ATOM	666	CB	LEU	A	109	30.316	16.182	22.280	1.00	24.30	C
ATOM	667	CG	LEU	A	109	31.003	16.770	23.483	1.00	25.72	C
ATOM	668	CD1	LEU	A	109	31.426	18.185	23.137	1.00	26.28	C
ATOM	669	CD2	LEU	A	109	30.097	16.820	24.677	1.00	25.67	N
ATOM	670	N	PHE	A	110	27.794	14.427	20.988	1.00	24.52	C
ATOM	671	CA	PHE	A	110	27.019	14.004	19.822	1.00	22.36	C
ATOM	672	C	PHE	A	110	25.996	15.079	19.586	1.00	21.47	O
ATOM	673	O	PHE	A	110	25.618	15.777	20.525	1.00	21.05	C
ATOM	674	CB	PHE	A	110	26.227	12.725	20.075	1.00	21.69	C
ATOM	675	CG	PHE	A	110	27.133	11.561	20.318	1.00	23.01	C
ATOM	676	CD1	PHE	A	110	27.676	10.892	19.238	1.00	24.43	C
ATOM	677	CD2	PHE	A	110	27.506	11.243	21.597	1.00	21.68	C
ATOM	678	CE1	PHE	A	110	28.614	9.897	19.463	1.00	24.92	C
ATOM	679	CE2	PHE	A	110	28.460	10.282	21.798	1.00	22.08	C
ATOM	680	CZ	PHE	A	110	29.017	9.597	20.746	1.00	23.51	N
ATOM	681	N	THR	A	111	25.557	15.239	18.339	1.00	20.40	C
ATOM	682	CA	THR	A	111	24.422	16.102	18.047	1.00	19.58	C
ATOM	683	C	THR	A	111	23.175	15.367	18.473	1.00	15.81	O
ATOM	684	O	THR	A	111	23.239	14.150	18.603	1.00	18.63	C
ATOM	685	CB	THR	A	111	24.305	16.421	16.578	1.00	19.96	O
ATOM	686	OG1	THR	A	111	24.145	15.178	15.907	1.00	21.91	C
ATOM	687	CG2	THR	A	111	25.487	17.252	16.118	1.00	23.08	N
ATOM	688	N	PRO	A	112	22.030	15.982	18.688	1.00	15.89	C
ATOM	689	CA	PRO	A	112	20.783	15.254	18.984	1.00	16.41	C
ATOM	690	C	PRO	A	112	20.500	14.089	18.025	1.00	17.10	O
ATOM	691	O	PRO	A	112	20.329	12.954	18.431	1.00	18.32	C
ATOM	692	CB	PRO	A	112	19.794	16.375	18.870	1.00	13.89	C
ATOM	693	CG	PRO	A	112	20.581	17.559	19.386	1.00	14.36	C
ATOM	694	CD	PRO	A	112	21.876	17.424	18.685	1.00	12.46	N
ATOM	695	N	GLU	A	113	20.564	14.321	16.728	1.00	20.22	C
ATOM	696	CA	GLU	A	113	20.393	13.303	15.737	1.00	24.11	C
ATOM	697	C	GLU	A	113	21.371	12.143	15.864	1.00	24.55	O
ATOM	698	O	GLU	A	113	20.963	10.982	15.866	1.00	25.38	C
ATOM	699	CB	GLU	A	113	20.539	13.991	14.420	1.00	29.66	C
ATOM	700	CG	GLU	A	113	20.432	13.029	13.250	1.00	41.26	C
ATOM	701	CD	GLU	A	113	21.253	13.476	12.042	1.00	49.84	C
ATOM	702	OE1	GLU	A	113	22.475	13.694	12.197	1.00	52.84	O
ATOM	703	OE2	GLU	A	113	20.662	13.586	10.949	1.00	55.78	N
ATOM	704	N	GLU	A	114	22.663	12.384	16.033	1.00	24.48	C
ATOM	705	CA	GLU	A	114	23.594	11.291	16.198	1.00	22.26	C
ATOM	706	C	GLU	A	114	23.398	10.486	17.471	1.00	22.80	O
ATOM	707	O	GLU	A	114	23.564	9.256	17.494	1.00	23.87	C
ATOM	708	CB	GLU	A	114	24.979	11.857	16.198	1.00	26.15	C
ATOM	709	CG	GLU	A	114	25.362	12.534	14.897	1.00	32.62	C
ATOM	710	CD	GLU	A	114	26.719	13.225	15.002	1.00	38.61	C
ATOM	711	OE1	GLU	A	114	26.860	14.093	15.867	1.00	41.67	O
ATOM	712	OE2	GLU	A	114	27.646	12.893	14.242	1.00	42.28	N
ATOM	713	N	PHE	A	115	23.035	11.181	18.558	1.00	21.59	C
ATOM	714	CA	PHE	A	115	22.812	10.544	19.850	1.00	19.30	C
ATOM	715	C	PHE	A	115	21.601	9.645	19.667	1.00	17.06	O
ATOM	716	O	PHE	A	115	21.555	8.527	20.165	1.00	17.46	C
ATOM	717	CB	PHE	A	115	22.586	11.623	20.972	1.00	16.68	C
ATOM	718	CG	PHE	A	115	22.148	11.018	22.298	1.00	13.67	C
ATOM	719	CD1	PHE	A	115	20.820	10.679	22.520	1.00	15.42	C
ATOM	720	CD2	PHE	A	115	23.081	10.752	23.261	1.00	15.56	C
ATOM	721	CE1	PHE	A	115	20.412	10.003	23.650	1.00	16.48	C
ATOM	722	CE2	PHE	A	115	22.674	10.136	24.429	1.00	17.36	C
ATOM	723	CZ	PHE	A	115	21.351	9.750	24.617	1.00	18.29	C
ATOM	724	N	PHE	A	116	20.581	10.135	18.981	1.00	18.67	N

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FIGURE 8A-23

ATOM	725	CA	PHE	A	116	19.401	9.327	18.860	1.00	18.51	C
ATOM	726	C	PHE	A	116	19.510	8.196	17.854	1.00	22.03	C
ATOM	727	O	PHE	A	116	18.768	7.213	17.892	1.00	22.83	O
ATOM	728	CB	PHE	A	116	18.204	10.195	18.687	1.00	19.13	C
ATOM	729	CG	PHE	A	116	17.735	10.764	20.021	1.00	19.41	C
ATOM	730	CD1	PHE	A	116	17.159	9.924	20.952	1.00	19.08	C
ATOM	731	CD2	PHE	A	116	17.991	12.079	20.343	1.00	19.60	C
ATOM	732	CE1	PHE	A	116	16.911	10.381	22.214	1.00	18.67	C
ATOM	733	CE2	PHE	A	116	17.747	12.528	21.619	1.00	21.95	C
ATOM	734	CZ	PHE	A	116	17.218	11.674	22.550	1.00	19.99	C
ATOM	735	N	ARG	A	117	20.510	8.249	16.986	1.00	22.43	N
ATOM	736	CA	ARG	A	117	20.822	7.134	16.123	1.00	21.98	C
ATOM	737	C	ARG	A	117	21.453	6.076	16.971	1.00	19.70	C
ATOM	738	O	ARG	A	117	21.039	4.946	16.841	1.00	22.56	O
ATOM	739	CB	ARG	A	117	21.769	7.623	15.052	1.00	27.63	C
ATOM	740	CG	ARG	A	117	22.329	6.596	14.082	1.00	36.33	C
ATOM	741	CD	ARG	A	117	23.135	7.255	12.971	1.00	43.02	C
ATOM	742	NE	ARG	A	117	22.296	8.207	12.239	1.00	49.61	N
ATOM	743	CZ	ARG	A	117	22.704	9.468	12.008	1.00	54.02	C
ATOM	744	NH1	ARG	A	117	23.915	9.867	12.474	1.00	53.58	N
ATOM	745	NH2	ARG	A	117	21.899	10.314	11.313	1.00	53.56	N
ATOM	746	N	ILE	A	118	22.394	6.348	17.874	1.00	19.56	N
ATOM	747	CA	ILE	A	118	22.944	5.328	18.746	1.00	18.66	C
ATOM	748	C	ILE	A	118	21.888	4.776	19.673	1.00	19.62	C
ATOM	749	O	ILE	A	118	21.887	3.579	19.933	1.00	21.23	O
ATOM	750	CB	ILE	A	118	24.054	5.970	19.533	1.00	21.60	C
ATOM	751	CG1	ILE	A	118	25.121	6.479	18.593	1.00	22.63	C
ATOM	752	CG2	ILE	A	118	24.665	5.002	20.534	1.00	22.20	C
ATOM	753	CD1	ILE	A	118	26.178	7.330	19.285	1.00	23.90	C
ATOM	754	N	PHE	A	119	20.971	5.619	20.180	1.00	20.06	N
ATOM	755	CA	PHE	A	119	19.827	5.124	20.943	1.00	21.07	C
ATOM	756	C	PHE	A	119	18.940	4.182	20.141	1.00	21.06	C
ATOM	757	O	PHE	A	119	18.720	3.075	20.600	1.00	22.31	O
ATOM	758	CB	PHE	A	119	19.001	6.253	21.590	1.00	18.55	C
ATOM	759	CG	PHE	A	119	17.726	5.856	22.342	1.00	18.55	C
ATOM	760	CD1	PHE	A	119	16.517	5.708	21.673	1.00	17.37	C
ATOM	761	CD2	PHE	A	119	17.736	5.715	23.718	1.00	21.09	C
ATOM	762	CE1	PHE	A	119	15.348	5.439	22.351	1.00	16.37	C
ATOM	763	CE2	PHE	A	119	16.555	5.448	24.404	1.00	19.97	C
ATOM	764	CZ	PHE	A	119	15.369	5.311	23.721	1.00	19.81	C
ATOM	765	N	ASN	A	120	18.426	4.507	18.957	1.00	22.51	N
ATOM	766	CA	ASN	A	120	17.567	3.577	18.222	1.00	23.92	C
ATOM	767	C	ASN	A	120	18.284	2.316	17.841	1.00	25.82	C
ATOM	768	O	ASN	A	120	17.653	1.274	17.841	1.00	26.73	O
ATOM	769	CB	ASN	A	120	16.912	4.179	16.996	1.00	20.96	C
ATOM	770	CG	ASN	A	120	15.857	5.195	17.377	1.00	24.90	C
ATOM	771	OD1	ASN	A	120	14.852	4.877	18.020	1.00	30.44	O
ATOM	772	ND2	ASN	A	120	16.044	6.458	17.023	1.00	26.09	N
ATOM	773	N	ARG	A	121	19.605	2.390	17.632	1.00	29.29	N
ATOM	774	CA	ARG	A	121	20.447	1.234	17.314	1.00	32.15	C
ATOM	775	C	ARG	A	121	20.686	0.283	18.503	1.00	32.13	C
ATOM	776	O	ARG	A	121	20.652	-0.949	18.369	1.00	32.27	O
ATOM	777	CB	ARG	A	121	21.752	1.846	16.891	1.00	36.26	C
ATOM	778	CG	ARG	A	121	22.606	0.988	16.001	1.00	42.80	C
ATOM	779	CD	ARG	A	121	24.066	1.304	16.288	1.00	45.46	C
ATOM	780	NE	ARG	A	121	24.730	0.026	16.469	1.00	49.59	N
ATOM	781	CZ	ARG	A	121	25.603	-0.473	15.599	1.00	47.62	C
ATOM	782	NH1	ARG	A	121	26.106	0.291	14.622	1.00	50.56	N
ATOM	783	NH2	ARG	A	121	25.907	-1.764	15.692	1.00	41.39	N
ATOM	784	N	SER	A	122	20.925	0.856	19.695	1.00	29.65	N

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FIGURE 8A-24

ATOM	785	CA	SER	A	122	20.981	0.077	20.908	1.00	27.73	C
ATOM	786	C	SER	A	122	19.643	-0.555	21.201	1.00	27.23	C
ATOM	787	O	SER	A	122	19.603	-1.652	21.716	1.00	28.27	O
ATOM	788	CB	SER	A	122	21.388	0.942	22.071	1.00	25.31	C
ATOM	789	OG	SER	A	122	22.619	1.543	21.726	1.00	25.19	O
ATOM	790	N	ILE	A	123	18.530	0.087	20.884	1.00	29.27	N
ATOM	791	CA	ILE	A	123	17.210	-0.453	21.140	1.00	31.25	C
ATOM	792	C	ILE	A	123	16.972	-1.618	20.207	1.00	32.43	C
ATOM	793	O	ILE	A	123	16.522	-2.672	20.637	1.00	32.75	O
ATOM	794	CB	ILE	A	123	16.129	0.661	20.973	1.00	33.20	C
ATOM	795	CG1	ILE	A	123	16.103	1.685	22.130	1.00	35.29	C
ATOM	796	CG2	ILE	A	123	14.739	0.181	20.629	1.00	33.87	C
ATOM	797	CD1	ILE	A	123	16.243	1.313	23.627	1.00	32.91	C
ATOM	798	N	ASP	A	124	17.325	-1.466	18.937	1.00	35.41	N
ATOM	799	CA	ASP	A	124	17.064	-2.502	17.973	1.00	38.41	C
ATOM	800	C	ASP	A	124	17.902	-3.728	18.170	1.00	38.55	C
ATOM	801	O	ASP	A	124	17.386	-4.820	17.960	1.00	39.71	O
ATOM	802	CB	ASP	A	124	17.074	-1.951	16.562	1.00	43.19	C
ATOM	803	CG	ASP	A	124	15.763	-1.179	16.387	1.00	51.27	C
ATOM	804	OD1	ASP	A	124	14.700	-1.790	16.620	1.00	56.07	O
ATOM	805	OD2	ASP	A	124	15.784	0.020	16.039	1.00	54.65	O
ATOM	806	N	ALA	A	125	19.102	-3.546	18.739	1.00	37.63	N
ATOM	807	CA	ALA	A	125	20.039	-4.621	18.983	1.00	37.10	C
ATOM	808	C	ALA	A	125	19.555	-5.682	19.944	1.00	39.02	C
ATOM	809	O	ALA	A	125	20.250	-6.667	20.151	1.00	40.94	O
ATOM	810	CB	ALA	A	125	21.321	-4.035	19.500	1.00	35.16	C
ATOM	811	N	PHE	A	126	18.374	-5.538	20.549	1.00	41.54	N
ATOM	812	CA	PHE	A	126	17.774	-6.599	21.363	1.00	45.13	C
ATOM	813	C	PHE	A	126	16.837	-7.482	20.578	1.00	47.39	C
ATOM	814	O	PHE	A	126	16.711	-8.660	20.900	1.00	48.19	O
ATOM	815	CB	PHE	A	126	16.971	-6.099	22.571	1.00	45.19	C
ATOM	816	CG	PHE	A	126	17.791	-5.456	23.683	1.00	44.53	C
ATOM	817	CD1	PHE	A	126	18.239	-4.150	23.568	1.00	43.63	C
ATOM	818	CD2	PHE	A	126	18.073	-6.184	24.815	1.00	44.69	C
ATOM	819	CE1	PHE	A	126	18.960	-3.565	24.576	1.00	41.80	C
ATOM	820	CE2	PHE	A	126	18.800	-5.597	25.822	1.00	43.70	C
ATOM	821	CZ	PHE	A	126	19.238	-4.295	25.700	1.00	43.96	C
ATOM	822	N	LYS	A	127	16.128	-6.898	19.600	1.00	50.61	N
ATOM	823	CA	LYS	A	127	15.283	-7.656	18.679	1.00	53.56	C
ATOM	824	C	LYS	A	127	16.149	-8.640	17.856	1.00	55.43	C
ATOM	825	O	LYS	A	127	16.038	-9.876	17.922	1.00	57.14	O
ATOM	826	CB	LYS	A	127	14.546	-6.638	17.764	1.00	51.56	C
ATOM	827	N	ASP	A	128	17.077	-8.036	17.105	1.00	57.96	N
ATOM	828	CA	ASP	A	128	18.105	-8.734	16.356	1.00	59.25	C
ATOM	829	C	ASP	A	128	19.292	-9.249	17.190	1.00	59.16	C
ATOM	830	O	ASP	A	128	20.461	-8.894	17.008	1.00	58.89	O
ATOM	831	CB	ASP	A	128	18.492	-7.915	15.062	1.00	61.00	C
ATOM	832	CG	ASP	A	128	18.868	-6.421	15.036	1.00	61.70	C
ATOM	833	OD1	ASP	A	128	20.024	-6.078	15.330	1.00	63.63	O
ATOM	834	OD2	ASP	A	128	18.015	-5.603	14.667	1.00	61.66	O
ATOM	835	N	PHE	A	129	18.967	-10.151	18.118	1.00	59.49	N
ATOM	836	CA	PHE	A	129	19.969	-10.719	19.002	1.00	61.20	C
ATOM	837	C	PHE	A	129	20.411	-12.103	18.503	1.00	61.55	C
ATOM	838	O	PHE	A	129	19.596	-12.979	18.179	1.00	61.67	O
ATOM	839	CB	PHE	A	129	19.410	-10.801	20.440	1.00	64.40	C
ATOM	840	CG	PHE	A	129	20.326	-10.282	21.561	1.00	67.62	C
ATOM	841	CD1	PHE	A	129	21.642	-10.721	21.686	1.00	68.55	C
ATOM	842	CD2	PHE	A	129	19.847	-9.338	22.473	1.00	69.51	C
ATOM	843	CE1	PHE	A	129	22.464	-10.192	22.672	1.00	68.84	C
ATOM	844	CE2	PHE	A	129	20.665	-8.823	23.472	1.00	68.79	C

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FIGURE 8A-25

ATOM	845	CZ	PHE	A	129	21.976	-9.245	23.561	1.00	69.80
ATOM	846	N	VAL	A	130	21.737	-12.294	18.417	1.00	60.68
ATOM	847	CA	VAL	A	130	22.337	-13.577	18.041	1.00	60.72
ATOM	848	C	VAL	A	130	23.459	-13.949	19.040	1.00	59.57
ATOM	849	O	VAL	A	130	24.157	-13.076	19.597	1.00	58.08
ATOM	850	CB	VAL	A	130	22.937	-13.560	16.582	1.00	60.98
ATOM	851	CG1	VAL	A	130	23.051	-15.001	16.068	1.00	60.93
ATOM	852	CG2	VAL	A	130	22.229	-12.635	15.579	1.00	58.32
ATOM	853	N	VAL	A	131	23.635	-15.277	19.213	1.00	57.03
ATOM	854	CA	VAL	A	131	24.634	-15.872	20.101	1.00	54.98
ATOM	855	C	VAL	A	131	26.059	-15.336	19.950	1.00	53.17
ATOM	856	O	VAL	A	131	26.547	-15.173	18.839	1.00	51.72
ATOM	857	CB	VAL	A	131	24.563	-17.411	19.950	1.00	55.34
ATOM	858	CG1	VAL	A	131	25.611	-18.162	20.780	1.00	55.30
ATOM	859	CG2	VAL	A	131	23.145	-17.893	20.297	1.00	54.41
ATOM	860	N	ALA	A	132	26.660	-15.027	21.117	1.00	52.91
ATOM	861	CA	ALA	A	132	28.022	-14.512	21.293	1.00	52.69
ATOM	862	C	ALA	A	132	29.161	-15.433	20.860	1.00	53.47
ATOM	863	O	ALA	A	132	30.250	-15.019	20.445	1.00	52.96
ATOM	864	CB	ALA	A	132	28.268	-14.176	22.771	1.00	48.84
ATOM	865	N	SER	A	133	28.899	-16.725	21.000	1.00	55.81
ATOM	866	CA	SER	A	133	29.812	-17.748	20.533	1.00	58.09
ATOM	867	C	SER	A	133	29.744	-17.881	19.005	1.00	59.46
ATOM	868	O	SER	A	133	30.726	-18.259	18.343	1.00	61.98
ATOM	869	CB	SER	A	133	29.348	-19.047	21.161	1.00	59.31
ATOM	870	N	GLU	A	134	28.556	-17.536	18.469	1.00	58.84
ATOM	871	CA	GLU	A	134	28.251	-17.530	17.031	1.00	57.10
ATOM	872	C	GLU	A	134	28.550	-16.218	16.298	1.00	54.08
ATOM	873	O	GLU	A	134	28.319	-16.114	15.094	1.00	50.66
ATOM	874	CB	GLU	A	134	26.768	-17.808	16.761	1.00	58.33
ATOM	875	CG	GLU	A	134	26.269	-19.189	17.121	1.00	61.93
ATOM	876	CD	GLU	A	134	24.955	-19.558	16.436	1.00	65.28
ATOM	877	OE1	GLU	A	134	24.056	-18.711	16.294	1.00	64.83
ATOM	878	OE2	GLU	A	134	24.853	-20.726	16.034	1.00	68.18
ATOM	879	N	THR	A	135	28.999	-15.169	16.988	1.00	52.70
ATOM	880	CA	THR	A	135	29.366	-13.953	16.291	1.00	51.61
ATOM	881	C	THR	A	135	30.896	-13.856	16.192	1.00	51.35
ATOM	882	O	THR	A	135	31.549	-14.721	15.580	1.00	52.93
ATOM	883	CB	THR	A	135	28.621	-12.683	16.830	1.00	49.31
ATOM	884	OG1	THR	A	135	29.039	-12.514	18.171	1.00	49.65
ATOM	885	CG2	THR	A	135	27.108	-12.772	16.767	1.00	48.16
ATOM	886	N	SER	A	136	31.473	-12.828	16.825	1.00	50.88
ATOM	887	CA	SER	A	136	32.885	-12.502	16.714	1.00	49.48
ATOM	888	C	SER	A	136	33.422	-12.163	18.121	1.00	47.44
ATOM	889	O	SER	A	136	32.624	-12.000	19.056	1.00	46.14
ATOM	890	CB	SER	A	136	32.966	-11.306	15.767	1.00	50.00
ATOM	891	OG	SER	A	136	32.146	-11.504	14.615	1.00	52.41
ATOM	892	N	ASP	A	137	34.760	-12.051	18.314	1.00	44.90
ATOM	893	CA	ASP	A	137	35.366	-11.578	19.566	1.00	40.01
ATOM	894	C	ASP	A	137	35.037	-10.093	19.850	1.00	36.45
ATOM	895	O	ASP	A	137	34.105	-9.570	19.228	1.00	35.34
ATOM	896	CB	ASP	A	137	36.879	-11.949	19.641	1.00	40.10
ATOM	897	CG	ASP	A	137	37.915	-11.197	18.783	1.00	44.69
ATOM	898	OD1	ASP	A	137	37.617	-10.121	18.252	1.00	46.41
ATOM	899	OD2	ASP	A	137	39.056	-11.661	18.648	1.00	46.87
ATOM	900	N	CYS	A	138	35.702	-9.337	20.741	1.00	32.95
ATOM	901	CA	CYS	A	138	35.263	-7.982	21.014	1.00	31.28
ATOM	902	C	CYS	A	138	36.311	-6.919	20.838	1.00	30.73
ATOM	903	O	CYS	A	138	36.233	-5.825	21.414	1.00	31.32
ATOM	904	CB	CYS	A	138	34.557	-7.854	22.361	1.00	32.08

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FIGURE 8A-26

ATOM	905	SG	CYS	A	138	32.988	-8.777	22.463	1.00	37.40	S
ATOM	906	N	VAL	A	139	37.258	-7.242	19.954	1.00	30.63	N
ATOM	907	CA	VAL	A	139	38.333	-6.318	19.599	1.00	29.74	C
ATOM	908	C	VAL	A	139	38.151	-5.898	18.168	1.00	28.81	C
ATOM	909	O	VAL	A	139	37.830	-6.734	17.342	1.00	27.95	O
ATOM	910	CB	VAL	A	139	39.769	-6.915	19.600	1.00	28.99	C
ATOM	911	CG1	VAL	A	139	40.717	-5.884	20.195	1.00	29.64	C
ATOM	912	CG2	VAL	A	139	39.889	-8.307	20.143	1.00	26.32	C
ATOM	913	N	VAL	A	140	38.424	-4.646	17.840	1.00	31.00	N
ATOM	914	CA	VAL	A	140	38.442	-4.247	16.459	1.00	34.50	C
ATOM	915	C	VAL	A	140	39.899	-4.167	16.020	1.00	36.64	C
ATOM	916	O	VAL	A	140	40.406	-5.059	15.323	1.00	39.48	O
ATOM	917	CB	VAL	A	140	37.758	-2.914	16.217	1.00	36.55	C
ATOM	918	CG1	VAL	A	140	37.417	-2.900	14.747	1.00	36.42	C
ATOM	919	CG2	VAL	A	140	36.594	-2.569	17.119	1.00	34.81	C
ATOM	920	N	SER	A	141	40.566	-3.136	16.529	1.00	37.83	N
ATOM	921	CA	SER	A	141	41.905	-2.682	16.123	1.00	41.81	C
ATOM	922	C	SER	A	141	41.936	-1.563	15.056	1.00	42.37	C
ATOM	923	O	SER	A	141	43.035	-1.174	14.685	1.00	43.60	O
ATOM	924	CB	SER	A	141	42.986	-3.811	15.889	1.00	42.08	C
ATOM	925	OG	SER	A	141	43.175	-4.693	17.008	1.00	38.01	O
TER	927		SER	A	141						
ATOM	928	N	ASN	B	11	2.666	37.382	21.946	1.00	65.93	N
ATOM	929	CA	ASN	B	11	1.945	36.256	22.556	1.00	66.50	C
ATOM	930	C	ASN	B	11	2.726	35.510	23.658	1.00	66.17	C
ATOM	931	O	ASN	B	11	3.559	34.641	23.372	1.00	66.24	O
ATOM	932	CB	ASN	B	11	1.488	35.204	21.515	1.00	66.50	C
ATOM	933	N	VAL	B	12	2.404	35.814	24.934	1.00	65.43	N
ATOM	934	CA	VAL	B	12	3.197	35.450	26.131	1.00	62.92	C
ATOM	935	C	VAL	B	12	3.195	33.985	26.631	1.00	60.27	C
ATOM	936	O	VAL	B	12	4.143	33.547	27.294	1.00	59.00	O
ATOM	937	CB	VAL	B	12	2.780	36.430	27.299	1.00	64.35	C
ATOM	938	CG1	VAL	B	12	1.408	36.086	27.935	1.00	63.94	C
ATOM	939	CG2	VAL	B	12	3.908	36.621	28.318	1.00	63.41	C
ATOM	940	N	LYS	B	13	2.125	33.208	26.374	1.00	56.82	N
ATOM	941	CA	LYS	B	13	2.071	31.821	26.800	1.00	51.85	C
ATOM	942	C	LYS	B	13	3.021	31.001	25.927	1.00	48.88	C
ATOM	943	O	LYS	B	13	3.595	30.003	26.380	1.00	49.33	O
ATOM	944	CB	LYS	B	13	0.640	31.283	26.675	1.00	52.25	C
ATOM	945	N	ASP	B	14	3.258	31.456	24.684	1.00	44.12	N
ATOM	946	CA	ASP	B	14	4.169	30.783	23.770	1.00	37.71	C
ATOM	947	C	ASP	B	14	5.662	30.978	24.040	1.00	31.42	C
ATOM	948	O	ASP	B	14	6.413	30.026	23.895	1.00	30.29	O
ATOM	949	CB	ASP	B	14	3.763	31.113	22.326	1.00	40.87	C
ATOM	950	CG	ASP	B	14	2.497	30.409	21.803	1.00	44.08	C
ATOM	951	OD1	ASP	B	14	1.832	29.636	22.531	1.00	44.87	O
ATOM	952	OD2	ASP	B	14	2.192	30.662	20.631	1.00	45.27	O
ATOM	953	N	VAL	B	15	6.165	32.130	24.468	1.00	25.72	N
ATOM	954	CA	VAL	B	15	7.545	32.234	24.906	1.00	24.93	C
ATOM	955	C	VAL	B	15	7.872	31.357	26.112	1.00	26.84	C
ATOM	956	O	VAL	B	15	8.935	30.739	26.124	1.00	29.81	O
ATOM	957	CB	VAL	B	15	7.914	33.670	25.178	1.00	22.45	C
ATOM	958	CG1	VAL	B	15	9.335	33.803	25.722	1.00	18.01	C
ATOM	959	CG2	VAL	B	15	7.730	34.435	23.895	1.00	21.89	C
ATOM	960	N	THR	B	16	6.962	31.275	27.104	1.00	27.60	N
ATOM	961	CA	THR	B	16	7.040	30.393	28.276	1.00	28.70	C
ATOM	962	C	THR	B	16	7.191	28.905	27.903	1.00	27.24	C
ATOM	963	O	THR	B	16	8.063	28.227	28.442	1.00	29.07	O
ATOM	964	CB	THR	B	16	5.797	30.649	29.237	1.00	30.92	C
ATOM	965	OG1	THR	B	16	5.967	31.920	29.887	1.00	30.85	O

FIGURE 8A-27

ATOM	966	CG2	THR	B	16	5.605	29.577	30.304	1.00	29.47	C
ATOM	967	N	LYS	B	17	6.385	28.387	26.979	1.00	24.02	N
ATOM	968	CA	LYS	B	17	6.508	27.042	26.455	1.00	25.48	C
ATOM	969	C	LYS	B	17	7.776	26.845	25.607	1.00	22.72	C
ATOM	970	O	LYS	B	17	8.397	25.806	25.690	1.00	22.89	O
ATOM	971	CB	LYS	B	17	5.235	26.851	25.662	1.00	29.47	C
ATOM	972	CG	LYS	B	17	5.047	25.479	25.076	1.00	36.80	C
ATOM	973	CD	LYS	B	17	3.820	25.460	24.129	1.00	40.47	C
ATOM	974	CE	LYS	B	17	3.432	24.008	23.742	1.00	42.23	C
ATOM	975	NZ	LYS	B	17	4.518	23.260	23.099	1.00	40.28	N
ATOM	976	N	LEU	B	18	8.223	27.840	24.836	1.00	21.80	N
ATOM	977	CA	LEU	B	18	9.489	27.797	24.148	1.00	19.84	C
ATOM	978	C	LEU	B	18	10.608	27.757	25.151	1.00	19.53	C
ATOM	979	O	LEU	B	18	11.425	26.868	24.985	1.00	22.71	O
ATOM	980	CB	LEU	B	18	9.660	28.989	23.206	1.00	17.63	C
ATOM	981	CG	LEU	B	18	10.954	29.148	22.479	1.00	13.25	C
ATOM	982	CD1	LEU	B	18	11.216	27.956	21.627	1.00	16.15	C
ATOM	983	CD2	LEU	B	18	10.895	30.338	21.606	1.00	13.19	C
ATOM	984	N	VAL	B	19	10.670	28.606	26.187	1.00	17.49	N
ATOM	985	CA	VAL	B	19	11.713	28.547	27.193	1.00	15.59	C
ATOM	986	C	VAL	B	19	11.708	27.199	27.912	1.00	16.76	O
ATOM	987	O	VAL	B	19	12.763	26.598	28.121	1.00	18.54	C
ATOM	988	CB	VAL	B	19	11.587	29.741	28.170	1.00	15.79	C
ATOM	989	CG1	VAL	B	19	12.566	29.662	29.308	1.00	13.19	C
ATOM	990	CG2	VAL	B	19	11.922	31.014	27.489	1.00	12.62	C
ATOM	991	N	ALA	B	20	10.533	26.655	28.232	1.00	17.26	N
ATOM	992	CA	ALA	B	20	10.415	25.384	28.918	1.00	17.20	C
ATOM	993	C	ALA	B	20	10.866	24.235	28.075	1.00	20.20	C
ATOM	994	O	ALA	B	20	11.185	23.166	28.578	1.00	22.02	O
ATOM	995	CB	ALA	B	20	8.972	25.064	29.185	1.00	18.25	C
ATOM	996	N	ASN	B	21	10.854	24.390	26.763	1.00	22.32	N
ATOM	997	CA	ASN	B	21	11.373	23.351	25.920	1.00	21.93	C
ATOM	998	C	ASN	B	21	12.711	23.661	25.314	1.00	21.34	C
ATOM	999	O	ASN	B	21	13.114	22.930	24.441	1.00	23.28	O
ATOM	1000	CB	ASN	B	21	10.378	23.022	24.873	1.00	26.17	C
ATOM	1001	CG	ASN	B	21	9.256	22.250	25.531	1.00	31.77	C
ATOM	1002	OD1	ASN	B	21	9.352	21.054	25.813	1.00	30.41	O
ATOM	1003	ND2	ASN	B	21	8.168	22.955	25.820	1.00	34.22	N
ATOM	1004	N	LEU	B	22	13.455	24.675	25.727	1.00	20.84	N
ATOM	1005	CA	LEU	B	22	14.825	24.880	25.285	1.00	18.95	C
ATOM	1006	C	LEU	B	22	15.754	24.358	26.359	1.00	19.14	C
ATOM	1007	O	LEU	B	22	15.428	24.560	27.526	1.00	19.71	O
ATOM	1008	CB	LEU	B	22	15.097	26.380	25.022	1.00	17.41	C
ATOM	1009	CG	LEU	B	22	14.510	27.035	23.750	1.00	15.79	C
ATOM	1010	CD1	LEU	B	22	14.718	28.544	23.724	1.00	13.61	C
ATOM	1011	CD2	LEU	B	22	15.120	26.381	22.517	1.00	14.80	C
ATOM	1012	N	PRO	B	23	16.903	23.701	26.091	1.00	18.35	N
ATOM	1013	CA	PRO	B	23	17.831	23.260	27.130	1.00	17.51	C
ATOM	1014	C	PRO	B	23	18.329	24.418	28.008	1.00	17.87	C
ATOM	1015	O	PRO	B	23	18.703	25.449	27.473	1.00	18.03	O
ATOM	1016	CB	PRO	B	23	18.908	22.619	26.307	1.00	13.87	C
ATOM	1017	CG	PRO	B	23	18.299	22.223	25.002	1.00	12.84	C
ATOM	1018	CD	PRO	B	23	17.457	23.421	24.762	1.00	14.01	C
ATOM	1019	N	LYS	B	24	18.327	24.340	29.347	1.00	18.87	N
ATOM	1020	CA	LYS	B	24	18.756	25.441	30.226	1.00	21.96	C
ATOM	1021	C	LYS	B	24	20.207	25.930	30.039	1.00	21.00	C
ATOM	1022	O	LYS	B	24	20.567	27.081	30.304	1.00	21.61	O
ATOM	1023	CB	LYS	B	24	18.456	25.044	31.703	1.00	23.68	C
ATOM	1024	CG	LYS	B	24	16.956	25.097	32.077	1.00	29.69	C
ATOM	1025	CD	LYS	B	24	16.544	24.407	33.429	1.00	34.88	C

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FIGURE 8A-28

ATOM	1026	CE	LYS	B	24	15.010	24.526	33.777	1.00	39.45	C
ATOM	1027	NZ	LYS	B	24	14.493	23.773	34.927	1.00	41.87	N
ATOM	1028	N	ASP	B	25	21.040	25.044	29.503	1.00	19.08	N
ATOM	1029	CA	ASP	B	25	22.440	25.350	29.263	1.00	20.79	C
ATOM	1030	C	ASP	B	25	22.758	25.601	27.789	1.00	19.77	C
ATOM	1031	O	ASP	B	25	23.907	25.469	27.373	1.00	20.06	O
ATOM	1032	CB	ASP	B	25	23.305	24.190	29.796	1.00	17.87	C
ATOM	1033	CG	ASP	B	25	23.063	22.836	29.175	1.00	20.81	O
ATOM	1034	OD1	ASP	B	25	21.975	22.598	28.651	1.00	22.64	N
ATOM	1035	OD2	ASP	B	25	23.964	21.991	29.214	1.00	24.79	C
ATOM	1036	N	TYR	B	26	21.753	25.866	26.950	1.00	19.06	C
ATOM	1037	CA	TYR	B	26	21.990	26.130	25.542	1.00	18.77	O
ATOM	1038	C	TYR	B	26	22.027	27.652	25.358	1.00	18.82	C
ATOM	1039	O	TYR	B	26	21.066	28.358	25.655	1.00	19.57	C
ATOM	1040	CB	TYR	B	26	20.900	25.477	24.712	1.00	16.23	C
ATOM	1041	CG	TYR	B	26	21.007	25.766	23.228	1.00	19.16	C
ATOM	1042	CD1	TYR	B	26	22.034	25.216	22.492	1.00	20.33	C
ATOM	1043	CD2	TYR	B	26	20.097	26.629	22.632	1.00	19.21	C
ATOM	1044	CE1	TYR	B	26	22.125	25.531	21.150	1.00	19.71	C
ATOM	1045	CE2	TYR	B	26	20.180	26.936	21.294	1.00	18.86	O
ATOM	1046	CZ	TYR	B	26	21.184	26.356	20.565	1.00	21.21	C
ATOM	1047	OH	TYR	B	26	21.209	26.560	19.204	1.00	23.57	O
HETATM	1048	N	MSE	B	27	23.136	28.207	24.891	1.00	18.02	N
HETATM	1049	CA	MSE	B	27	23.249	29.645	24.886	1.00	20.01	C
HETATM	1050	C	MSE	B	27	22.894	30.253	23.553	1.00	20.43	C
HETATM	1051	O	MSE	B	27	23.319	29.791	22.493	1.00	22.74	O
HETATM	1052	CB	MSE	B	27	24.648	30.070	25.309	1.00	21.80	C
HETATM	1053	CG	MSE	B	27	25.179	29.494	26.646	1.00	24.25	SE
HETATM	1054	SE	MSE	B	27	24.219	29.995	28.260	1.00	30.76	C
HETATM	1055	CE	MSE	B	27	24.936	31.691	28.317	1.00	17.91	N
ATOM	1056	N	ILE	B	28	22.071	31.294	23.642	1.00	21.17	C
ATOM	1057	CA	ILE	B	28	21.690	32.092	22.507	1.00	20.03	C
ATOM	1058	C	ILE	B	28	22.501	33.383	22.470	1.00	20.64	O
ATOM	1059	O	ILE	B	28	22.545	34.162	23.403	1.00	19.83	C
ATOM	1060	CB	ILE	B	28	20.168	32.289	22.522	1.00	19.56	C
ATOM	1061	CG1	ILE	B	28	19.489	30.935	22.719	1.00	14.81	C
ATOM	1062	CG2	ILE	B	28	19.653	32.893	21.195	1.00	17.30	N
ATOM	1063	CD1	ILE	B	28	17.993	31.054	22.978	1.00	14.38	C
ATOM	1064	N	THR	B	29	23.235	33.585	21.364	1.00	22.56	C
ATOM	1065	CA	THR	B	29	24.048	34.777	21.117	1.00	21.92	O
ATOM	1066	C	THR	B	29	23.167	35.926	20.723	1.00	21.18	C
ATOM	1067	O	THR	B	29	22.235	35.744	19.926	1.00	24.05	O
ATOM	1068	CB	THR	B	29	25.003	34.540	19.949	1.00	24.32	N
ATOM	1069	OG1	THR	B	29	25.751	33.393	20.310	1.00	26.19	C
ATOM	1070	CG2	THR	B	29	25.901	35.743	19.657	1.00	23.45	C
ATOM	1071	N	LEU	B	30	23.485	37.110	21.229	1.00	19.18	O
ATOM	1072	CA	LEU	B	30	22.694	38.278	20.928	1.00	19.42	C
ATOM	1073	C	LEU	B	30	23.612	39.444	21.123	1.00	20.84	C
ATOM	1074	O	LEU	B	30	24.251	39.604	22.155	1.00	22.59	C
ATOM	1075	CB	LEU	B	30	21.486	38.458	21.822	1.00	16.57	C
ATOM	1076	CG	LEU	B	30	20.712	39.739	21.692	1.00	17.65	N
ATOM	1077	CD1	LEU	B	30	19.907	39.690	20.405	1.00	15.54	C
ATOM	1078	CD2	LEU	B	30	19.875	40.004	22.946	1.00	14.12	C
ATOM	1079	N	LYS	B	31	23.641	40.271	20.085	1.00	21.41	O
ATOM	1080	CA	LYS	B	31	24.340	41.533	20.142	1.00	22.33	C
ATOM	1081	C	LYS	B	31	23.462	42.478	20.918	1.00	21.90	C
ATOM	1082	O	LYS	B	31	22.714	43.295	20.370	1.00	24.57	C
ATOM	1083	CB	LYS	B	31	24.642	42.093	18.754	1.00	21.18	C
ATOM	1084	CG	LYS	B	31	25.844	41.479	18.111	1.00	21.89	C
ATOM	1085	CD	LYS	B	31	25.551	41.360	16.647	1.00	29.30	C

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FIGURE 8A-29

ATOM	1086	CE	LYS	B	31	26.741	40.957	15.808	1.00	31.29
ATOM	1087	NZ	LYS	B	31	27.628	42.105	15.688	1.00	39.41
ATOM	1088	N	TYR	B	32	23.572	42.299	22.227	1.00	21.32
ATOM	1089	CA	TYR	B	32	22.800	43.101	23.138	1.00	19.60
ATOM	1090	C	TYR	B	32	23.198	44.586	22.981	1.00	19.96
ATOM	1091	O	TYR	B	32	24.384	44.940	22.977	1.00	20.37
ATOM	1092	CB	TYR	B	32	23.094	42.513	24.532	1.00	17.35
ATOM	1093	CG	TYR	B	32	22.621	43.373	25.710	1.00	17.26
ATOM	1094	CD1	TYR	B	32	21.298	43.297	26.107	1.00	15.20
ATOM	1095	CD2	TYR	B	32	23.490	44.280	26.299	1.00	14.00
ATOM	1096	CE1	TYR	B	32	20.851	44.149	27.086	1.00	13.12
ATOM	1097	CE2	TYR	B	32	23.013	45.166	27.227	1.00	14.39
ATOM	1098	CZ	TYR	B	32	21.702	45.070	27.606	1.00	13.82
ATOM	1099	OH	TYR	B	32	21.213	45.916	28.560	1.00	18.31
ATOM	1100	N	VAL	B	33	22.179	45.455	22.873	1.00	19.13
ATOM	1101	CA	VAL	B	33	22.376	46.889	22.818	1.00	19.34
ATOM	1102	C	VAL	B	33	22.478	47.489	24.223	1.00	22.86
ATOM	1103	O	VAL	B	33	21.487	47.535	24.979	1.00	23.26
ATOM	1104	CB	VAL	B	33	21.220	47.609	22.071	1.00	18.33
ATOM	1105	CG1	VAL	B	33	21.607	49.014	21.732	1.00	17.72
ATOM	1106	CG2	VAL	B	33	20.868	46.933	20.772	1.00	18.88
ATOM	1107	N	PRO	B	34	23.669	48.022	24.556	1.00	23.14
ATOM	1108	CA	PRO	B	34	23.950	48.685	25.814	1.00	25.98
ATOM	1109	C	PRO	B	34	22.991	49.844	26.052	1.00	27.87
ATOM	1110	O	PRO	B	34	22.782	50.697	25.173	1.00	28.20
ATOM	1111	CB	PRO	B	34	25.355	49.247	25.629	1.00	24.52
ATOM	1112	CG	PRO	B	34	25.947	48.454	24.514	1.00	23.81
ATOM	1113	CD	PRO	B	34	24.761	48.256	23.617	1.00	23.96
ATOM	1114	N	GLY	B	35	22.428	49.854	27.265	1.00	27.60
ATOM	1115	CA	GLY	B	35	21.544	50.919	27.694	1.00	26.85
ATOM	1116	C	GLY	B	35	20.103	50.509	27.809	1.00	26.95
ATOM	1117	O	GLY	B	35	19.314	51.234	28.392	1.00	27.06
HETATM	1118	N	MSE	B	36	19.736	49.361	27.277	1.00	27.66
HETATM	1119	CA	MSE	B	36	18.444	48.762	27.502	1.00	31.16
HETATM	1120	C	MSE	B	36	17.873	48.948	28.920	1.00	33.96
HETATM	1121	O	MSE	B	36	16.708	49.315	29.138	1.00	34.27
HETATM	1122	CB	MSE	B	36	18.679	47.299	27.225	1.00	34.63
HETATM	1123	CG	MSE	B	36	17.921	46.622	26.126	1.00	37.69
HETATM	1124	SE	MSE	B	36	16.954	45.030	26.682	1.00	48.87
HETATM	1125	CE	MSE	B	36	16.692	45.161	28.580	1.00	40.22
ATOM	1126	N	ASP	B	37	18.753	48.712	29.902	1.00	35.95
ATOM	1127	CA	ASP	B	37	18.421	48.828	31.303	1.00	37.28
ATOM	1128	C	ASP	B	37	18.228	50.272	31.758	1.00	38.57
ATOM	1129	O	ASP	B	37	17.189	50.545	32.368	1.00	42.23
ATOM	1130	CB	ASP	B	37	19.407	48.058	32.203	1.00	38.21
ATOM	1131	CG	ASP	B	37	20.907	48.280	32.005	1.00	42.18
ATOM	1132	OD1	ASP	B	37	21.288	49.092	31.150	1.00	44.69
ATOM	1133	OD2	ASP	B	37	21.709	47.641	32.708	1.00	43.60
ATOM	1134	N	VAL	B	38	19.111	51.237	31.458	1.00	36.46
ATOM	1135	CA	VAL	B	38	18.974	52.585	32.008	1.00	34.42
ATOM	1136	C	VAL	B	38	18.360	53.701	31.150	1.00	35.48
ATOM	1137	O	VAL	B	38	17.844	54.706	31.662	1.00	35.46
ATOM	1138	CB	VAL	B	38	20.314	53.047	32.623	1.00	33.96
ATOM	1139	CG1	VAL	B	38	20.656	52.110	33.757	1.00	33.39
ATOM	1140	CG2	VAL	B	38	21.452	53.127	31.638	1.00	30.40
ATOM	1141	N	LEU	B	39	18.466	53.536	29.826	1.00	34.58
ATOM	1142	CA	LEU	B	39	18.173	54.590	28.859	1.00	33.84
ATOM	1143	C	LEU	B	39	16.770	54.521	28.304	1.00	34.39
ATOM	1144	O	LEU	B	39	16.234	53.407	28.274	1.00	37.21
ATOM	1145	CB	LEU	B	39	19.106	54.513	27.672	1.00	31.59

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FIGURE 8A-30

ATOM	1146	CG	LEU	B	39	20.516	54.934	27.836	1.00	30.49	C
ATOM	1147	CD1	LEU	B	39	21.233	54.571	26.544	1.00	30.11	C
ATOM	1148	CD2	LEU	B	39	20.556	56.416	28.187	1.00	28.81	C
ATOM	1149	N	PRO	B	40	16.124	55.613	27.821	1.00	33.22	N
ATOM	1150	CA	PRO	B	40	14.743	55.564	27.336	1.00	32.18	C
ATOM	1151	C	PRO	B	40	14.595	54.656	26.104	1.00	31.61	C
ATOM	1152	O	PRO	B	40	15.515	54.575	25.295	1.00	32.07	O
ATOM	1153	CB	PRO	B	40	14.498	57.028	27.054	1.00	31.41	C
ATOM	1154	CG	PRO	B	40·	15.395	57.749	28.027	1.00	32.72	C
ATOM	1155	CD	PRO	B	40	16.655	56.977	27.813	1.00	33.34	C
ATOM	1156	N	SER	B	41	13.487	53.949	25.885	1.00	31.04	N
ATOM	1157	CA	SER	B	41	13.422	52.973	24.819	1.00	32.48	C
ATOM	1158	C	SER	B	41	13.785	53.436	23.428	1.00	32.31	C
ATOM	1159	O	SER	B	41	14.301	52.651	22.638	1.00	30.86	O
ATOM	1160	CB	SER	B	41	12.119	52.197	24.820	1.00	34.06	C
ATOM	1161	OG	SER	B	41	10.984	53.037	24.872	1.00	39.11	O
ATOM	1162	N	HIS	B	42	13.622	54.747	23.191	1.00	34.63	N
ATOM	1163	CA	HIS	B	42	13.911	55.363	21.888	1.00	36.02	C
ATOM	1164	C	HIS	B	42	15.396	55.300	21.511	1.00	36.52	C
ATOM	1165	O	HIS	B	42	15.780	55.228	20.327	1.00	34.40	O
ATOM	1166	CB	HIS	B	42	13.316	56.805	21.755	1.00	34.27	C
ATOM	1167	CG	HIS	B	42	13.946	57.935	22.576	1.00	34.59	C
ATOM	1168	ND1	HIS	B	42	13.588	58.408	23.772	1.00	36.14	N
ATOM	1169	CD2	HIS	B	42	15.013	58.687	22.154	1.00	32.00	C
ATOM	1170	CE1	HIS	B	42	14.381	59.396	24.117	1.00	32.43	C
ATOM	1171	NE2	HIS	B	42	15.227	59.539	23.124	1.00	35.02	N
ATOM	1172	N	CYS	B	43	16.177	55.249	22.615	1.00	35.96	N
ATOM	1173	CA	CYS	B	43	17.627	55.122	22.565	1.00	35.90	C
ATOM	1174	C	CYS	B	43	18.176	53.799	22.054	1.00	32.86	C
ATOM	1175	O	CYS	B	43	19.347	53.782	21.649	1.00	33.40	O
ATOM	1176	CB	CYS	B	43	18.339	55.448	23.910·	1.00	40.38	C
ATOM	1177	SG	CYS	B	43	18.099	57.127	24.542	1.00	45.68	S
ATOM	1178	N	TRP	B	44	17.380	52.707	22.075	1.00	29.25	N
ATOM	1179	CA	TRP	B	44	17.913	51.374	21.831	1.00	25.51	C
ATOM	1180	C	TRP	B	44	17.009	50.463	21.066	1.00	24.22	C
ATOM	1181	O	TRP	B	44	17.544	49.594	20.406	1.00	26.02	O
ATOM	1182	CB	TRP	B	44	18.375	50.661	23.113	1.00	21.99	C
ATOM	1183	CG	TRP	B	44	17.351	50.644	24.234	1.00	20.34	C
ATOM	1184	CD1	TRP	B	44	17.361	51.632	25.183	1.00	18.11	C
ATOM	1185	CD2	TRP	B	44	16.297	49.745	24.363	1.00	19.23	C
ATOM	1186	NE1	TRP	B	44	16.293	51.390	25.908	1.00	19.12	N
ATOM	1187	CE2	TRP	B	44	15.635	50.281	25.471	1.00	18.20	C
ATOM	1188	CE3	TRP	B	44	15.892	48.551	23.795	1.00	15.22	C
ATOM	1189	CZ2	TRP	B	44	14.532	49.622	26.000	1.00	14.99	C
ATOM	1190	CZ3	TRP	B	44	14.805	47.897	24.324	1.00	13.45	C
ATOM	1191	CH2	TRP	B	44	14.130	48.434	25.405	1.00	15.50	C
ATOM	1192	N	ILE	B	45	15.680	50.626	21.096	1.00	24.85	N
ATOM	1193	CA	ILE	B	45	14.726	49.656	20.539	1.00	25.50	C
ATOM	1194	C	ILE	B	45	14.926	49.254	19.094	1.00	26.34	C
ATOM	1195	O	ILE	B	45	14.724	48.086	18.762	1.00	28.11	O
ATOM	1196	CB	ILE	B	45	13.231	50.055	20.773	1.00	26.28	C
ATOM	1197	CG1	ILE	B	45	12.358	48.838	20.592	1.00	24.31	C
ATOM	1198	CG2	ILE	B	45	12.716	51.206	19.885	1.00	25.51	C
ATOM	1199	CD1	ILE	B	45	12.688	47.633	21.486	1.00	19.41	C
ATOM	1200	N	SER	B	46	15.336	50.233	18.274	1.00	28.06	N
ATOM	1201	CA	SER	B	46	15.623	50.071	16.851	1.00	28.67	C
ATOM	1202	C	SER	B	46	16.739	49.059	16.553	1.00	27.51	C
ATOM	1203	O	SER	B	46	16.558	48.113	15.773	1.00	26.90	O
ATOM	1204	CB	SER	B	46	15.933	51.472	16.250	1.00	28.71	C
ATOM	1205	OG	SER	B	46	16.259	51.414	14.871	1.00	31.35	C

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FIGURE 8A-31

ATOM	1206	N	GLU	B	47	17.902	49.210	17.203	1.00	26.77
ATOM	1207	CA	GLU	B	47	18.910	48.173	17.142	1.00	27.22
ATOM	1208	C	GLU	B	47	18.555	46.912	17.906	1.00	23.80
ATOM	1209	O	GLU	B	47	19.011	45.850	17.513	1.00	24.85
ATOM	1210	CB	GLU	B	47	20.209	48.703	17.683	1.00	30.36
ATOM	1211	CG	GLU	B	47	21.460	47.909	17.269	1.00	31.64
ATOM	1212	CD	GLU	B	47	21.718	47.840	15.774	1.00	31.93
ATOM	1213	OE1	GLU	B	47	21.267	48.726	15.034	1.00	32.82
ATOM	1214	OE2	GLU	B	47	22.391	46.892	15.366	1.00	31.60
HETATM	1215	N	MSE	B	48	17.739	46.958	18.958	1.00	23.65
HETATM	1216	CA	MSE	B	48	17.401	45.755	19.709	1.00	21.94
HETATM	1217	C	MSE	B	48	16.511	44.916	18.837	1.00	22.24
HETATM	1218	O	MSE	B	48	16.819	43.732	18.731	1.00	24.91
HETATM	1219	CB	MSE	B	48	16.783	46.061	21.080	1.00	22.86
HETATM	1220	CG	MSE	B	48	16.875	44.981	22.173	1.00	24.51
HETATM	1221	SE	MSE	B	48	18.597	44.203	22.615	1.00	30.61
HETATM	1222	CE	MSE	B	48	17.982	42.661	21.922	1.00	26.74
ATOM	1223	N	VAL	B	49	15.506	45.445	18.110	1.00	21.88
ATOM	1224	CA	VAL	B	49	14.661	44.597	17.276	1.00	20.25
ATOM	1225	C	VAL	B	49	15.387	43.973	16.098	1.00	20.18
ATOM	1226	O	VAL	B	49	15.120	42.815	15.780	1.00	22.62
ATOM	1227	CB	VAL	B	49	13.351	45.252	16.813	1.00	23.22
ATOM	1228	CG1	VAL	B	49	12.455	45.562	17.992	1.00	24.62
ATOM	1229	CG2	VAL	B	49	13.551	46.527	16.025	1.00	23.30
ATOM	1230	N	VAL	B	50	16.363	44.655	15.484	1.00	19.52
ATOM	1231	CA	VAL	B	50	17.179	44.087	14.408	1.00	19.02
ATOM	1232	C	VAL	B	50	18.005	42.916	14.897	1.00	19.73
ATOM	1233	O	VAL	B	50	18.091	41.872	14.232	1.00	19.76
ATOM	1234	CB	VAL	B	50	18.110	45.171	13.808	1.00	18.29
ATOM	1235	CG1	VAL	B	50	19.181	44.607	12.925	1.00	16.52
ATOM	1236	CG2	VAL	B	50	17.290	46.136	13.024	1.00	18.74
ATOM	1237	N	GLN	B	51	18.617	43.151	16.064	1.00	17.95
ATOM	1238	CA	GLN	B	51	19.447	42.130	16.677	1.00	18.39
ATOM	1239	C	GLN	B	51	18.645	40.938	17.084	1.00	16.66
ATOM	1240	O	GLN	B	51	19.056	39.827	16.830	1.00	18.39
ATOM	1241	CB	GLN	B	51	20.264	42.655	17.851	1.00	18.87
ATOM	1242	CG	GLN	B	51	21.265	43.713	17.440	1.00	18.55
ATOM	1243	CD	GLN	B	51	22.253	43.283	16.370	1.00	23.83
ATOM	1244	OE1	GLN	B	51	22.400	42.141	15.918	1.00	23.92
ATOM	1245	NE2	GLN	B	51	23.019	44.265	15.958	1.00	27.04
ATOM	1246	N	LEU	B	52	17.481	41.149	17.652	1.00	16.16
ATOM	1247	CA	LEU	B	52	16.615	40.053	18.010	1.00	17.66
ATOM	1248	C	LEU	B	52	16.106	39.302	16.810	1.00	18.23
ATOM	1249	O	LEU	B	52	16.012	38.080	16.844	1.00	18.09
ATOM	1250	CB	LEU	B	52	15.412	40.576	18.771	1.00	19.12
ATOM	1251	CG	LEU	B	52	15.665	40.840	20.232	1.00	20.87
ATOM	1252	CD1	LEU	B	52	14.609	41.767	20.734	1.00	20.47
ATOM	1253	CD2	LEU	B	52	15.692	39.553	21.037	1.00	21.69
ATOM	1254	N	SER	B	53	15.797	40.014	15.717	1.00	20.42
ATOM	1255	CA	SER	B	53	15.410	39.376	14.469	1.00	18.47
ATOM	1256	C	SER	B	53	16.491	38.428	13.973	1.00	18.27
ATOM	1257	O	SER	B	53	16.259	37.257	13.692	1.00	17.53
ATOM	1258	CB	SER	B	53	15.188	40.496	13.523	1.00	21.19
ATOM	1259	OG	SER	B	53	14.858	39.866	12.317	1.00	22.45
ATOM	1260	N	ASP	B	54	17.729	38.892	13.962	1.00	21.01
ATOM	1261	CA	ASP	B	54	18.811	38.060	13.483	1.00	25.15
ATOM	1262	C	ASP	B	54	19.040	36.841	14.339	1.00	24.43
ATOM	1263	O	ASP	B	54	19.279	35.764	13.782	1.00	24.72
ATOM	1264	CB	ASP	B	54	20.170	38.731	13.462	1.00	32.20
ATOM	1265	CG	ASP	B	54	20.366	40.017	12.671	1.00	44.10

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FIGURE 8A-32

ATOM	1266	OD1	ASP	B	54	19.508	40.411	11.838	1.00	48.06
ATOM	1267	OD2	ASP	B	54	21.429	40.630	12.924	1.00	50.40
ATOM	1268	N	SER	B	55	19.025	37.009	15.674	1.00	21.94
ATOM	1269	CA	SER	B	55	19.197	35.872	16.589	1.00	21.29
ATOM	1270	C	SER	B	55	18.036	34.884	16.516	1.00	19.86
ATOM	1271	O	SER	B	55	18.259	33.675	16.567	1.00	20.94
ATOM	1272	CB	SER	B	55	19.356	36.295	18.052	1.00	18.68
ATOM	1273	OG	SER	B	55	20.384	37.208	18.406	1.00	18.26
ATOM	1274	N	LEU	B	56	16.789	35.362	16.374	1.00	20.32
ATOM	1275	CA	LEU	B	56	15.647	34.453	16.343	1.00	20.44
ATOM	1276	C	LEU	B	56	15.628	33.735	15.025	1.00	21.16
ATOM	1277	O	LEU	B	56	15.299	32.552	14.968	1.00	20.64
ATOM	1278	CB	LEU	B	56	14.335	35.169	16.568	1.00	19.08
ATOM	1279	CG	LEU	B	56	13.967	35.545	17.993	1.00	19.76
ATOM	1280	CD1	LEU	B	56	12.809	36.497	18.033	1.00	18.12
ATOM	1281	CD2	LEU	B	56	13.621	34.308	18.773	1.00	17.63
ATOM	1282	N	THR	B	57	16.081	34.451	13.984	1.00	22.55
ATOM	1283	CA	THR	B	57	16.144	33.901	12.624	1.00	23.77
ATOM	1284	C	THR	B	57	17.169	32.775	12.599	1.00	25.31
ATOM	1285	O	THR	B	57	16.904	31.674	12.109	1.00	28.36
ATOM	1286	CB	THR	B	57	16.420	35.019	11.581	1.00	22.83
ATOM	1287	OG1	THR	B	57	15.245	35.800	11.520	1.00	20.28
ATOM	1288	CG2	THR	B	57	16.608	34.496	10.209	1.00	22.98
ATOM	1289	N	ASP	B	58	18.331	32.975	13.229	1.00	27.29
ATOM	1290	CA	ASP	B	58	19.328	31.934	13.394	1.00	25.16
ATOM	1291	C	ASP	B	58	18.874	30.781	14.238	1.00	22.74
ATOM	1292	O	ASP	B	58	19.128	29.640	13.909	1.00	20.50
ATOM	1293	CB	ASP	B	58	20.510	32.549	14.059	1.00	32.90
ATOM	1294	CG	ASP	B	58	21.367	33.343	13.098	1.00	40.22
ATOM	1295	OD1	ASP	B	58	21.635	32.807	11.999	1.00	47.28
ATOM	1296	OD2	ASP	B	58	21.780	34.468	13.458	1.00	42.79
ATOM	1297	N	LEU	B	59	18.174	31.090	15.328	1.00	22.88
ATOM	1298	CA	LEU	B	59	17.597	30.066	16.166	1.00	22.01
ATOM	1299	C	LEU	B	59	16.596	29.206	15.391	1.00	22.75
ATOM	1300	O	LEU	B	59	16.642	27.981	15.498	1.00	24.25
ATOM	1301	CB	LEU	B	59	16.984	30.711	17.389	1.00	21.26
ATOM	1302	CG	LEU	B	59	16.544	29.703	18.408	1.00	21.05
ATOM	1303	CD1	LEU	B	59	17.733	28.955	19.020	1.00	20.13
ATOM	1304	CD2	LEU	B	59	15.718	30.419	19.413	1.00	20.68
ATOM	1305	N	LEU	B	60	15.729	29.754	14.537	1.00	22.30
ATOM	1306	CA	LEU	B	60	14.838	28.912	13.776	1.00	21.18
ATOM	1307	C	LEU	B	60	15.559	27.884	12.897	1.00	24.69
ATOM	1308	O	LEU	B	60	15.084	26.761	12.702	1.00	27.59
ATOM	1309	CB	LEU	B	60	13.949	29.829	12.982	1.00	20.34
ATOM	1310	CG	LEU	B	60	12.805	29.256	12.208	1.00	15.11
ATOM	1311	CD1	LEU	B	60	11.775	28.689	13.124	1.00	14.00
ATOM	1312	CD2	LEU	B	60	12.216	30.351	11.405	1.00	15.62
ATOM	1313	N	ASP	B	61	16.768	28.142	12.405	1.00	28.19
ATOM	1314	CA	ASP	B	61	17.425	27.134	11.587	1.00	31.01
ATOM	1315	C	ASP	B	61	17.898	25.925	12.380	1.00	30.42
ATOM	1316	O	ASP	B	61	18.293	24.903	11.836	1.00	30.78
ATOM	1317	CB	ASP	B	61	18.486	27.766	10.638	1.00	40.38
ATOM	1318	CG	ASP	B	61	20.011	27.910	10.913	1.00	49.60
ATOM	1319	OD1	ASP	B	61	20.632	27.086	11.630	1.00	52.10
ATOM	1320	OD2	ASP	B	61	20.602	28.852	10.340	1.00	54.11
ATOM	1321	N	LYS	B	62	17.841	26.023	13.706	1.00	29.72
ATOM	1322	CA	LYS	B	62	18.282	24.972	14.586	1.00	26.53
ATOM	1323	C	LYS	B	62	17.227	23.920	14.754	1.00	26.40
ATOM	1324	O	LYS	B	62	17.553	22.835	15.224	1.00	28.09
ATOM	1325	CB	LYS	B	62	18.655	25.534	15.953	1.00	25.89

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FIGURE 8A-33

ATOM	1326	CG	LYS	B	62	19.865	26.451	15.996	1.00	24.99	C
ATOM	1327	CD	LYS	B	62	21.053	25.810	15.308	1.00	26.66	C
ATOM	1328	CE	LYS	B	62	22.198	26.806	15.251	1.00	28.58	N
ATOM	1329	NZ	LYS	B	62	21.868	27.957	14.431	1.00	34.52	N
ATOM	1330	N	PHE	B	63	15.986	24.225	14.389	1.00	26.48	C
ATOM	1331	CA	PHE	B	63	14.862	23.316	14.568	1.00	29.27	C
ATOM	1332	C	PHE	B	63	14.293	22.916	13.220	1.00	31.78	O
ATOM	1333	O	PHE	B	63	14.573	23.581	12.227	1.00	34.39	C
ATOM	1334	CB	PHE	B	63	13.744	23.920	15.427	1.00	24.13	C
ATOM	1335	CG	PHE	B	63	14.261	24.236	16.809	1.00	23.83	C
ATOM	1336	CD1	PHE	B	63	14.269	23.261	17.761	1.00	20.94	C
ATOM	1337	CD2	PHE	B	63	14.811	25.488	17.066	1.00	25.00	C
ATOM	1338	CE1	PHE	B	63	14.872	23.535	18.964	1.00	23.54	C
ATOM	1339	CE2	PHE	B	63	15.444	25.741	18.263	1.00	22.33	N
ATOM	1340	CZ	PHE	B	63	15.467	24.752	19.211	1.00	21.46	C
ATOM	1341	N	SER	B	64	13.565	21.791	13.203	1.00	35.96	O
ATOM	1342	CA	SER	B	64	12.847	21.251	12.047	1.00	41.24	C
ATOM	1343	C	SER	B	64	11.362	21.237	12.401	1.00	44.87	O
ATOM	1344	O	SER	B	64	11.045	21.210	13.593	1.00	45.47	N
ATOM	1345	CB	SER	B	64	13.299	19.810	11.723	1.00	39.81	C
ATOM	1346	OG	SER	B	64	14.690	19.659	11.441	1.00	41.15	C
ATOM	1347	N	ASN	B	65	10.393	21.257	11.464	1.00	50.28	O
ATOM	1348	CA	ASN	B	65	8.980	21.293	11.878	1.00	53.31	C
ATOM	1349	C	ASN	B	65	8.304	19.970	12.291	1.00	53.88	C
ATOM	1350	O	ASN	B	65	8.619	18.877	11.815	1.00	53.27	O
ATOM	1351	CB	ASN	B	65	8.137	22.121	10.899	1.00	55.21	N
ATOM	1352	CG	ASN	B	65	6.847	22.674	11.525	1.00	58.28	C
ATOM	1353	OD1	ASN	B	65	5.829	22.845	10.846	1.00	62.80	C
ATOM	1354	ND2	ASN	B	65	6.802	22.997	12.821	1.00	58.83	O
ATOM	1355	N	ILE	B	66	7.402	20.111	13.274	1.00	55.78	N
ATOM	1356	CA	ILE	B	66	6.604	19.028	13.857	1.00	58.20	C
ATOM	1357	C	ILE	B	66	5.128	19.413	13.732	1.00	59.99	C
ATOM	1358	O	ILE	B	66	4.679	20.439	14.266	1.00	59.98	O
ATOM	1359	CB	ILE	B	66	6.916	18.864	15.373	1.00	58.00	C
ATOM	1360	CG1	ILE	B	66	8.393	18.635	15.673	1.00	56.77	C
ATOM	1361	CG2	ILE	B	66	6.119	17.713	15.950	1.00	58.43	C
ATOM	1362	CD1	ILE	B	66	8.729	18.733	17.169	1.00	53.61	N
ATOM	1363	N	SER	B	67	4.387	18.545	13.027	1.00	62.59	C
ATOM	1364	CA	SER	B	67	2.945	18.687	12.803	1.00	65.18	C
ATOM	1365	C	SER	B	67	2.049	18.114	13.935	1.00	66.39	O
ATOM	1366	O	SER	B	67	1.110	17.339	13.725	1.00	68.18	C
ATOM	1367	CB	SER	B	67	2.632	18.133	11.385	1.00	65.71	O
ATOM	1368	OG	SER	B	67	3.288	16.912	10.995	1.00	67.79	N
ATOM	1369	N	GLU	B	68	2.307	18.549	15.184	1.00	66.59	C
ATOM	1370	CA	GLU	B	68	1.793	17.929	16.415	1.00	65.52	C
ATOM	1371	C	GLU	B	68	0.895	18.865	17.238	1.00	66.78	O
ATOM	1372	O	GLU	B	68	-0.333	18.715	17.307	1.00	67.15	C
ATOM	1373	CB	GLU	B	68	2.977	17.471	17.301	1.00	66.40	C
ATOM	1374	CG	GLU	B	68	2.568	17.163	18.743	1.00	67.84	C
ATOM	1375	CD	GLU	B	68	3.745	16.736	19.622	1.00	69.12	O
ATOM	1376	OE1	GLU	B	68	4.931	16.661	19.119	1.00	70.46	O
ATOM	1377	OE2	GLU	B	68	3.552	16.451	20.865	1.00	71.34	N
ATOM	1378	N	GLY	B	69	1.582	19.807	17.897	1.00	65.16	C
ATOM	1379	CA	GLY	B	69	1.015	20.935	18.626	1.00	63.26	C
ATOM	1380	C	GLY	B	69	2.019	22.049	18.382	1.00	60.63	O
ATOM	1381	O	GLY	B	69	2.666	22.081	17.308	1.00	60.82	N
ATOM	1382	N	LEU	B	70	2.179	22.963	19.355	1.00	57.50	C
ATOM	1383	CA	LEU	B	70	3.254	23.950	19.225	1.00	53.07	C
ATOM	1384	C	LEU	B	70	4.610	23.233	19.244	1.00	50.38	O
ATOM	1385	O	LEU	B	70	4.879	22.324	20.040	1.00	53.95	

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FIGURE 8A-34

ATOM	1386	CB	LEU	B	70	3.243	25.033	20.295	1.00	52.74	C
ATOM	1387	CG	LEU	B	70	2.243	26.184	20.332	1.00	54.01	C
ATOM	1388	CD1	LEU	B	70	2.326	26.991	19.014	1.00	54.05	C
ATOM	1389	CD2	LEU	B	70	0.834	25.683	20.698	1.00	55.75	C
ATOM	1390	N	SER	B	71	5.437	23.543	18.271	1.00	43.22	N
ATOM	1391	CA	SER	B	71	6.788	23.107	18.347	1.00	37.10	C
ATOM	1392	C	SER	B	71	7.676	24.348	18.452	1.00	35.41	C
ATOM	1393	O	SER	B	71	7.223	25.469	18.195	1.00	34.32	O
ATOM	1394	CB	SER	B	71	7.030	22.242	17.147	1.00	36.36	C
ATOM	1395	OG	SER	B	71	6.753	22.899	15.934	1.00	36.82	O
ATOM	1396	N	ASN	B	72	8.946	24.206	18.876	1.00	33.26	N
ATOM	1397	CA	ASN	B	72	9.888	25.327	18.974	1.00	28.70	C
ATOM	1398	C	ASN	B	72	10.013	26.017	17.631	1.00	25.92	C
ATOM	1399	O	ASN	B	72	10.086	27.234	17.591	1.00	25.46	O
ATOM	1400	CB	ASN	B	72	11.281	24.862	19.462	1.00	28.21	C
ATOM	1401	CG	ASN	B	72	11.365	24.292	20.880	1.00	26.47	C
ATOM	1402	OD1	ASN	B	72	10.592	24.638	21.764	1.00	25.38	O
ATOM	1403	ND2	ASN	B	72	12.284	23.373	21.160	1.00	26.66	N
ATOM	1404	N	TYR	B	73	9.968	25.221	16.547	1.00	26.29	N
ATOM	1405	CA	TYR	B	73	9.940	25.723	15.179	1.00	26.54	C
ATOM	1406	C	TYR	B	73	8.760	26.639	14.993	1.00	23.80	C
ATOM	1407	O	TYR	B	73	8.967	27.809	14.726	1.00	27.19	O
ATOM	1408	CB	TYR	B	73	9.881	24.631	14.075	1.00	28.15	C
ATOM	1409	CG	TYR	B	73	10.162	25.129	12.647	1.00	28.60	C
ATOM	1410	CD1	TYR	B	73	9.210	25.828	11.901	1.00	29.58	C
ATOM	1411	CD2	TYR	B	73	11.426	24.929	12.122	1.00	30.26	C
ATOM	1412	CE1	TYR	B	73	9.566	26.391	10.690	1.00	29.50	C
ATOM	1413	CE2	TYR	B	73	11.783	25.467	10.898	1.00	31.02	C
ATOM	1414	CZ	TYR	B	73	10.855	26.215	10.209	1.00	32.38	C
ATOM	1415	OH	TYR	B	73	11.245	26.802	9.014	1.00	36.91	O
ATOM	1416	N	SER	B	74	7.535	26.185	15.145	1.00	23.20	N
ATOM	1417	CA	SER	B	74	6.402	27.077	15.028	1.00	24.27	C
ATOM	1418	C	SER	B	74	6.449	28.270	15.935	1.00	23.26	C
ATOM	1419	O	SER	B	74	6.039	29.360	15.572	1.00	25.85	O
ATOM	1420	CB	SER	B	74	5.156	26.342	15.357	1.00	25.27	C
ATOM	1421	OG	SER	B	74	5.173	25.254	14.460	1.00	32.42	O
ATOM	1422	N	ILE	B	75	6.958	28.120	17.146	1.00	25.08	N
ATOM	1423	CA	ILE	B	75	6.913	29.248	18.057	1.00	23.59	C
ATOM	1424	C	ILE	B	75	7.908	30.294	17.620	1.00	21.89	C
ATOM	1425	O	ILE	B	75	7.509	31.437	17.519	1.00	21.19	O
ATOM	1426	CB	ILE	B	75	7.150	28.785	19.482	1.00	23.07	C
ATOM	1427	CG1	ILE	B	75	5.984	27.956	19.962	1.00	23.49	C
ATOM	1428	CG2	ILE	B	75	7.272	29.985	20.397	1.00	22.81	C
ATOM	1429	CD1	ILE	B	75	6.254	27.309	21.343	1.00	21.59	C
ATOM	1430	N	ILE	B	76	9.149	29.881	17.347	1.00	21.79	N
ATOM	1431	CA	ILE	B	76	10.226	30.789	16.994	1.00	22.16	C
ATOM	1432	C	ILE	B	76	9.830	31.465	15.705	1.00	23.36	C
ATOM	1433	O	ILE	B	76	9.898	32.679	15.673	1.00	26.09	O
ATOM	1434	CB	ILE	B	76	11.611	30.123	16.831	1.00	21.17	C
ATOM	1435	CG1	ILE	B	76	12.075	29.444	18.092	1.00	19.74	C
ATOM	1436	CG2	ILE	B	76	12.661	31.169	16.489	1.00	18.62	C
ATOM	1437	CD1	ILE	B	76	13.143	28.388	17.846	1.00	17.66	C
ATOM	1438	N	ASP	B	77	9.353	30.734	14.702	1.00	23.97	N
ATOM	1439	CA	ASP	B	77	8.866	31.293	13.456	1.00	25.97	C
ATOM	1440	C	ASP	B	77	7.856	32.411	13.657	1.00	26.70	C
ATOM	1441	O	ASP	B	77	8.065	33.525	13.187	1.00	28.84	O
ATOM	1442	CB	ASP	B	77	8.223	30.179	12.680	1.00	28.57	C
ATOM	1443	CG	ASP	B	77	8.018	30.507	11.212	1.00	32.25	C
ATOM	1444	OD1	ASP	B	77	8.957	31.036	10.598	1.00	34.07	O
ATOM	1445	OD2	ASP	B	77	6.927	30.224	10.704	1.00	32.50	C

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FIGURE 8A-35

ATOM	1446	N	LYS	B	78	6.797	32.211	14.443	1.00	28.77	N
ATOM	1447	CA	LYS	B	78	5.891	33.285	14.868	1.00	28.31	C
ATOM	1448	C	LYS	B	78	6.596	34.463	15.571	1.00	26.90	C
ATOM	1449	O	LYS	B	78	6.221	35.629	15.449	1.00	26.22	O
ATOM	1450	CB	LYS	B	78	4.861	32.589	15.762	1.00	32.30	C
ATOM	1451	CG	LYS	B	78	3.767	33.491	16.290	1.00	41.29	C
ATOM	1452	CD	LYS	B	78	2.746	32.676	17.100	1.00	49.72	C
ATOM	1453	CE	LYS	B	78	1.564	33.546	17.666	1.00	53.37	C
ATOM	1454	NZ	LYS	B	78	0.551	32.773	18.406	1.00	54.23	N
ATOM	1455	N	LEU	B	79	7.663	34.218	16.330	1.00	25.35	N
ATOM	1456	CA	LEU	B	79	8.352	35.299	17.007	1.00	23.52	C
ATOM	1457	C	LEU	B	79	9.151	36.141	16.063	1.00	22.42	C
ATOM	1458	O	LEU	B	79	9.249	37.348	16.219	1.00	20.72	O
ATOM	1459	CB	LEU	B	79	9.292	34.752	18.074	1.00	23.66	C
ATOM	1460	CG	LEU	B	79	8.739	33.917	19.241	1.00	21.39	C
ATOM	1461	CD1	LEU	B	79	9.823	33.698	20.260	1.00	17.54	C
ATOM	1462	CD2	LEU	B	79	7.579	34.608	19.911	1.00	21.67	C
ATOM	1463	N	VAL	B	80	9.727	35.426	15.094	1.00	25.43	N
ATOM	1464	CA	VAL	B	80	10.474	35.983	13.952	1.00	25.77	C
ATOM	1465	C	VAL	B	80	9.566	36.918	13.200	1.00	25.42	O
ATOM	1466	O	VAL	B	80	9.948	38.052	12.971	1.00	26.43	C
ATOM	1467	CB	VAL	B	80	10.989	34.920	12.949	1.00	24.61	C
ATOM	1468	CG1	VAL	B	80	11.693	35.588	11.801	1.00	26.74	C
ATOM	1469	CG2	VAL	B	80	12.018	33.999	13.521	1.00	24.19	N
ATOM	1470	N	ASN	B	81	8.352	36.466	12.893	1.00	27.82	C
ATOM	1471	CA	ASN	B	81	7.420	37.299	12.163	1.00	29.77	O
ATOM	1472	C	ASN	B	81	6.999	38.527	12.964	1.00	29.38	C
ATOM	1473	O	ASN	B	81	6.937	39.593	12.377	1.00	32.14	C
ATOM	1474	CB	ASN	B	81	6.221	36.505	11.562	1.00	31.24	O
ATOM	1475	CG	ASN	B	81	6.543	35.379	10.564	1.00	33.72	N
ATOM	1476	OD1	ASN	B	81	7.608	35.271	9.962	1.00	34.16	N
ATOM	1477	ND2	ASN	B	81	5.614	34.454	10.332	1.00	37.55	C
ATOM	1478	N	ILE	B	82	6.761	38.515	14.283	1.00	30.06	O
ATOM	1479	CA	ILE	B	82	6.418	39.713	15.057	1.00	27.77	C
ATOM	1480	C	ILE	B	82	7.591	40.672	15.019	1.00	28.50	C
ATOM	1481	O	ILE	B	82	7.388	41.866	14.826	1.00	30.63	C
ATOM	1482	CB	ILE	B	82	6.164	39.318	16.534	1.00	27.91	N
ATOM	1483	CG1	ILE	B	82	4.880	38.557	16.625	1.00	29.24	C
ATOM	1484	CG2	ILE	B	82	6.192	40.458	17.555	1.00	23.22	O
ATOM	1485	CD1	ILE	B	82	4.796	37.771	17.958	1.00	33.77	C
ATOM	1486	N	VAL	B	83	8.833	40.218	15.222	1.00	28.54	C
ATOM	1487	CA	VAL	B	83	9.884	41.192	15.413	1.00	28.60	N
ATOM	1488	C	VAL	B	83	10.348	41.752	14.061	1.00	32.57	C
ATOM	1489	O	VAL	B	83	10.849	42.878	13.989	1.00	32.81	O
ATOM	1490	CB	VAL	B	83	10.975	40.632	16.338	1.00	26.41	C
ATOM	1491	CG1	VAL	B	83	11.972	39.760	15.644	1.00	26.53	C
ATOM	1492	CG2	VAL	B	83	11.609	41.742	17.144	1.00	25.82	N
ATOM	1493	N	ASP	B	84	10.153	40.975	12.980	1.00	33.06	C
ATOM	1494	CA	ASP	B	84	10.383	41.446	11.632	1.00	34.79	C
ATOM	1495	C	ASP	B	84	9.332	42.450	11.205	1.00	34.82	O
ATOM	1496	O	ASP	B	84	9.665	43.271	10.357	1.00	36.49	C
ATOM	1497	CB	ASP	B	84	10.391	40.329	10.601	1.00	37.40	C
ATOM	1498	CG	ASP	B	84	11.732	39.649	10.403	1.00	41.65	O
ATOM	1499	OD1	ASP	B	84	12.767	40.242	10.726	1.00	45.61	O
ATOM	1500	OD2	ASP	B	84	11.746	38.524	9.895	1.00	45.89	N
ATOM	1501	N	ASP	B	85	8.101	42.430	11.753	1.00	33.73	C
ATOM	1502	CA	ASP	B	85	7.134	43.501	11.551	1.00	32.67	C
ATOM	1503	C	ASP	B	85	7.527	44.753	12.304	1.00	31.61	O
ATOM	1504	O	ASP	B	85	7.290	45.876	11.852	1.00	30.78	C
ATOM	1505	CB	ASP	B	85	5.689	43.092	11.967	1.00	36.31	C

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FIGURE 8A-36

ATOM	1506	CG	ASP	B	85	4.984	42.012	11.146	1.00	36.50	C
ATOM	1507	OD1	ASP	B	85	5.491	41.708	10.065	1.00	34.52	O
ATOM	1508	OD2	ASP	B	85	3.945	41.485	11.574	1.00	37.36	O
ATOM	1509	N	LEU	B	86	8.151	44.567	13.473	1.00	31.94	N
ATOM	1510	CA	LEU	B	86	8.695	45.686	14.241	1.00	29.00	C
ATOM	1511	C	LEU	B	86	9.945	46.335	13.646	1.00	27.01	C
ATOM	1512	O	LEU	B	86	10.158	47.536	13.788	1.00	25.07	O
ATOM	1513	CB	LEU	B	86	8.888	45.242	15.703	1.00	29.72	C
ATOM	1514	CG	LEU	B	86	7.630	44.973	16.544	1.00	29.69	C
ATOM	1515	CD1	LEU	B	86	7.934	44.246	17.825	1.00	29.68	C
ATOM	1516	CD2	LEU	B	86	6.938	46.265	16.914	1.00	29.39	C
ATOM	1517	N	VAL	B	87	10.774	45.550	12.962	1.00	26.28	N
ATOM	1518	CA	VAL	B	87	11.895	46.068	12.214	1.00	29.27	C
ATOM	1519	C	VAL	B	87	11.333	47.009	11.163	1.00	32.65	C
ATOM	1520	O	VAL	B	87	11.721	48.175	11.164	1.00	35.43	O
ATOM	1521	CB	VAL	B	87	12.725	44.966	11.523	1.00	28.93	C
ATOM	1522	CG1	VAL	B	87	13.789	45.570	10.630	1.00	25.59	C
ATOM	1523	CG2	VAL	B	87	13.417	44.036	12.521	1.00	30.50	C
ATOM	1524	N	GLU	B	88	10.392	46.534	10.325	1.00	34.28	N
ATOM	1525	CA	GLU	B	88	9.820	47.291	9.217	1.00	34.18	C
ATOM	1526	C	GLU	B	88	9.201	48.582	9.702	1.00	34.90	C
ATOM	1527	O	GLU	B	88	9.505	49.640	9.178	1.00	35.08	O
ATOM	1528	CB	GLU	B	88	8.789	46.446	8.468	1.00	34.62	C
ATOM	1529	CG	GLU	B	88	9.361	45.233	7.725	1.00	35.13	C
ATOM	1530	CD	GLU	B	88	8.360	44.218	7.145	1.00	37.81	C
ATOM	1531	OE1	GLU	B	88	7.241	44.088	7.653	1.00	39.42	O
ATOM	1532	OE2	GLU	B	88	8.696	43.539	6.176	1.00	38.59	O
ATOM	1533	N	CYS	B	89	8.402	48.520	10.754	1.00	37.74	N
ATOM	1534	CA	CYS	B	89	7.803	49.680	11.378	1.00	41.43	C
ATOM	1535	C	CYS	B	89	8.798	50.685	11.934	1.00	43.62	C
ATOM	1536	O	CYS	B	89	8.578	51.896	11.896	1.00	44.63	O
ATOM	1537	CB	CYS	B	89	6.875	49.166	12.472	1.00	43.51	C
ATOM	1538	SG	CYS	B	89	6.538	50.326	13.821	1.00	52.54	S
ATOM	1539	N	VAL	B	90	9.907	50.205	12.473	1.00	45.45	N
ATOM	1540	CA	VAL	B	90	10.919	51.096	13.007	1.00	48.36	C
ATOM	1541	C	VAL	B	90	11.787	51.723	11.909	1.00	49.57	C
ATOM	1542	O	VAL	B	90	12.399	52.768	12.121	1.00	50.61	O
ATOM	1543	CB	VAL	B	90	11.681	50.331	14.107	1.00	48.77	C
ATOM	1544	CG1	VAL	B	90	12.903	51.039	14.582	1.00	51.24	C
ATOM	1545	CG2	VAL	B	90	10.793	50.256	15.316	1.00	48.76	C
ATOM	1546	N	LYS	B	91	11.834	51.181	10.695	1.00	50.84	N
ATOM	1547	CA	LYS	B	91	12.492	51.870	9.600	1.00	52.46	C
ATOM	1548	C	LYS	B	91	11.615	52.881	8.847	1.00	53.71	C
ATOM	1549	O	LYS	B	91	12.139	53.730	8.127	1.00	52.07	O
ATOM	1550	CB	LYS	B	91	13.135	50.840	8.721	1.00	54.00	C
ATOM	1551	CG	LYS	B	91	14.290	50.209	9.508	1.00	59.12	C
ATOM	1552	CD	LYS	B	91	14.955	49.089	8.690	1.00	63.16	C
ATOM	1553	CE	LYS	B	91	16.176	48.420	9.367	1.00	66.55	C
ATOM	1554	NZ	LYS	B	91	16.631	47.252	8.605	1.00	68.43	N
ATOM	1555	N	GLU	B	92	10.283	52.858	9.066	1.00	56.63	N
ATOM	1556	CA	GLU	B	92	9.333	53.861	8.565	1.00	59.16	C
ATOM	1557	C	GLU	B	92	9.366	55.130	9.381	1.00	60.82	C
ATOM	1558	O	GLU	B	92	9.635	56.189	8.802	1.00	61.59	O
ATOM	1559	CB	GLU	B	92	7.852	53.434	8.599	1.00	60.60	C
ATOM	1560	CG	GLU	B	92	7.388	52.228	7.784	1.00	63.20	C
ATOM	1561	CD	GLU	B	92	7.621	52.275	6.273	1.00	66.00	C
ATOM	1562	OE1	GLU	B	92	7.843	53.369	5.709	1.00	65.65	O
ATOM	1563	OE2	GLU	B	92	7.564	51.187	5.667	1.00	67.41	O
ATOM	1564	N	ASN	B	93	9.061	54.977	10.698	1.00	62.57	N
ATOM	1565	CA	ASN	B	93	9.063	56.041	11.714	1.00	64.84	C

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FIGURE 8A-37

ATOM	1566	C	ASN	B	93	10.247	56.971	11.593	1.00	65.46	C
ATOM	1567	O	ASN	B	93	11.368	56.721	12.018	1.00	65.03	O
ATOM	1568	CB	ASN	B	93	9.069	55.511	13.153	1.00	63.55	C
ATOM	1569	N	SER	B	94	9.868	58.041	10.904	1.00	68.52	N
ATOM	1570	CA	SER	B	94	10.773	58.985	10.254	1.00	70.87	C
ATOM	1571	C	SER	B	94	11.391	60.076	11.141	1.00	71.17	C
ATOM	1572	O	SER	B	94	12.292	60.821	10.689	1.00	72.46	O
ATOM	1573	CB	SER	B	94	10.028	59.573	9.039	1.00	71.38	C
ATOM	1574	OG	SER	B	94	8.711	60.001	9.407	1.00	73.36	O
ATOM	1575	N	SER	B	95	10.923	60.135	12.415	1.00	68.97	N
ATOM	1576	CA	SER	B	95	11.564	60.953	13.424	1.00	68.06	C
ATOM	1577	C	SER	B	95	13.040	60.572	13.473	1.00	67.28	C
ATOM	1578	O	SER	B	95	13.457	59.458	13.839	1.00	64.89	O
ATOM	1579	CB	SER	B	95	10.932	60.795	14.794	1.00	68.06	C
ATOM	1580	OG	SER	B	95	11.441	61.800	15.670	1.00	69.36	O
ATOM	1581	N	LYS	B	96	13.755	61.565	12.916	1.00	66.92	N
ATOM	1582	CA	LYS	B	96	15.199	61.518	12.771	1.00	67.27	C
ATOM	1583	C	LYS	B	96	15.848	60.974	14.056	1.00	66.10	C
ATOM	1584	O	LYS	B	96	16.615	59.996	14.014	1.00	64.46	O
ATOM	1585	CB	LYS	B	96	15.699	62.948	12.478	1.00	67.07	C
ATOM	1586	N	ASP	B	97	15.289	61.560	15.147	1.00	64.54	N
ATOM	1587	CA	ASP	B	97	15.657	61.369	16.562	1.00	62.82	C
ATOM	1588	C	ASP	B	97	15.739	59.968	17.239	1.00	60.00	C
ATOM	1589	O	ASP	B	97	16.792	59.674	17.852	1.00	59.90	O
ATOM	1590	CB	ASP	B	97	14.689	62.230	17.394	1.00	63.85	C
ATOM	1591	N	LEU	B	98	14.638	59.137	17.174	1.00	53.67	N
ATOM	1592	CA	LEU	B	98	14.641	57.690	17.447	1.00	44.35	C
ATOM	1593	C	LEU	B	98	15.837	57.135	16.728	1.00	40.32	C
ATOM	1594	O	LEU	B	98	15.868	57.109	15.497	1.00	40.10	O
ATOM	1595	CB	LEU	B	98	13.389	56.996	16.916	1.00	41.21	C
ATOM	1596	CG	LEU	B	98	13.251	55.479	17.095	1.00	40.48	C
ATOM	1597	CD1	LEU	B	98	11.904	55.030	17.695	1.00	39.61	C
ATOM	1598	CD2	LEU	B	98	13.519	54.787	15.784	1.00	37.90	C
ATOM	1599	N	LYS	B	99	16.815	56.840	17.593	1.00	36.84	N
ATOM	1600	CA	LYS	B	99	18.171	56.457	17.229	1.00	35.08	C
ATOM	1601	C	LYS	B	99	18.141	55.218	16.365	1.00	34.40	C
ATOM	1602	O	LYS	B	99	17.600	54.164	16.712	1.00	34.91	O
ATOM	1603	CB	LYS	B	99	19.028	56.193	18.485	1.00	35.16	C
ATOM	1604	CG	LYS	B	99	20.550	56.058	18.286	1.00	37.24	C
ATOM	1605	CD	LYS	B	99	21.314	55.641	19.556	1.00	36.33	C
ATOM	1606	CE	LYS	B	99	22.817	55.994	19.594	1.00	38.98	C
ATOM	1607	NZ	LYS	B	99	23.617	55.657	18.428	1.00	38.67	N
ATOM	1608	N	LYS	B	100	18.689	55.387	15.174	1.00	34.28	N
ATOM	1609	CA	LYS	B	100	18.726	54.285	14.232	1.00	34.35	C
ATOM	1610	C	LYS	B	100	20.147	53.964	13.811	1.00	31.26	C
ATOM	1611	O	LYS	B	100	20.368	52.917	13.224	1.00	32.09	O
ATOM	1612	CB	LYS	B	100	17.832	54.592	13.044	1.00	36.01	C
ATOM	1613	CG	LYS	B	100	16.335	54.635	13.349	1.00	38.72	C
ATOM	1614	CD	LYS	B	100	15.782	55.851	12.617	1.00	43.22	C
ATOM	1615	CE	LYS	B	100	14.290	55.723	12.370	1.00	43.50	C
ATOM	1616	NZ	LYS	B	100	13.982	55.990	10.969	1.00	43.57	N
ATOM	1617	N	SER	B	101	21.120	54.814	14.159	1.00	29.00	C
ATOM	1618	CA	SER	B	101	22.529	54.614	13.871	1.00	28.55	C
ATOM	1619	C	SER	B	101	23.351	54.047	15.032	1.00	28.24	O
ATOM	1620	O	SER	B	101	23.732	54.783	15.943	1.00	31.98	C
ATOM	1621	CB	SER	B	101	23.049	55.977	13.473	1.00	27.88	C
ATOM	1622	OG	SER	B	101	24.459	55.979	13.457	1.00	27.09	N
ATOM	1623	N	PHE	B	102	23.680	52.766	15.077	1.00	27.56	C
ATOM	1624	CA	PHE	B	102	24.364	52.184	16.230	1.00	27.12	O
ATOM	1625	C	PHE	B	102	25.620	51.495	15.755	1.00	28.99	C

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FIGURE 8A-38

ATOM	1626	O	PHE	B	102	25.613	51.001	14.627	1.00	28.31
ATOM	1627	CB	PHE	B	102	23.538	51.127	16.945	1.00	22.35
ATOM	1628	CG	PHE	B	102	22.247	51.672	17.462	1.00	20.73
ATOM	1629	CD1	PHE	B	102	21.206	51.877	16.608	1.00	22.70
ATOM	1630	CD2	PHE	B	102	22.105	51.932	18.801	1.00	24.01
ATOM	1631	CE1	PHE	B	102	20.007	52.325	17.098	1.00	23.86
ATOM	1632	CE2	PHE	B	102	20.892	52.343	19.295	1.00	23.54
ATOM	1633	CZ	PHE	B	102	19.837	52.536	18.435	1.00	23.17
ATOM	1634	N	LYS	B	103	26.691	51.459	16.575	1.00	30.21
ATOM	1635	CA	LYS	B	103	27.823	50.595	16.284	1.00	30.86
ATOM	1636	C	LYS	B	103	27.374	49.171	16.550	1.00	32.14
ATOM	1637	O	LYS	B	103	26.583	48.957	17.472	1.00	33.74
ATOM	1638	CB	LYS	B	103	28.965	50.952	17.200	1.00	32.77
ATOM	1639	N	SER	B	104	27.788	48.202	15.720	1.00	32.95
ATOM	1640	CA	SER	B	104	27.284	46.825	15.805	1.00	33.85
ATOM	1641	C	SER	B	104	27.695	46.249	17.145	1.00	31.14
ATOM	1642	O	SER	B	104	28.891	46.121	17.418	1.00	32.16
ATOM	1643	CB	SER	B	104	27.812	45.908	14.692	1.00	36.29
ATOM	1644	OG	SER	B	104	28.690	46.589	13.784	1.00	44.97
ATOM	1645	N	PRO	B	105	26.737	45.950	18.023	1.00	28.62
ATOM	1646	CA	PRO	B	105	27.026	45.601	19.393	1.00	27.39
ATOM	1647	C	PRO	B	105	27.816	44.315	19.472	1.00	26.85
ATOM	1648	O	PRO	B	105	27.947	43.532	18.527	1.00	29.04
ATOM	1649	CB	PRO	B	105	25.668	45.476	19.982	1.00	26.67
ATOM	1650	CG	PRO	B	105	24.803	46.313	19.104	1.00	26.85
ATOM	1651	CD	PRO	B	105	25.308	45.910	17.747	1.00	26.48
ATOM	1652	N	GLU	B	106	28.426	44.160	20.628	1.00	27.12
ATOM	1653	CA	GLU	B	106	29.240	42.982	20.897	1.00	27.97
ATOM	1654	C	GLU	B	106	28.299	41.806	21.172	1.00	25.13
ATOM	1655	O	GLU	B	106	27.294	41.966	21.870	1.00	21.99
ATOM	1656	CB	GLU	B	106	30.140	43.258	22.105	1.00	30.05
ATOM	1657	CG	GLU	B	106	31.418	42.451	22.220	1.00	35.47
ATOM	1658	CD	GLU	B	106	32.045	42.483	23.613	1.00	40.01
ATOM	1659	OE1	GLU	B	106	32.162	43.570	24.198	1.00	41.10
ATOM	1660	OE2	GLU	B	106	32.431	41.409	24.102	1.00	42.35
ATOM	1661	N	PRO	B	107	28.564	40.640	20.578	1.00	23.74
ATOM	1662	CA	PRO	B	107	27.806	39.423	20.817	1.00	24.07
ATOM	1663	C	PRO	B	107	27.906	38.967	22.264	1.00	22.95
ATOM	1664	O	PRO	B	107	28.989	38.920	22.832	1.00	24.47
ATOM	1665	CB	PRO	B	107	28.437	38.439	19.837	1.00	24.75
ATOM	1666	CG	PRO	B	107	28.949	39.309	18.715	1.00	25.17
ATOM	1667	CD	PRO	B	107	29.556	40.448	19.512	1.00	24.46
ATOM	1668	N	ARG	B	108	26.765	38.677	22.884	1.00	22.39
ATOM	1669	CA	ARG	B	108	26.684	38.164	24.239	1.00	20.57
ATOM	1670	C	ARG	B	108	25.904	36.865	24.227	1.00	17.43
ATOM	1671	O	ARG	B	108	24.954	36.685	23.488	1.00	17.22
ATOM	1672	CB	ARG	B	108	26.064	39.155	25.256	1.00	20.10
ATOM	1673	CG	ARG	B	108	27.007	40.157	25.848	1.00	21.68
ATOM	1674	CD	ARG	B	108	26.321	41.144	26.778	1.00	25.69
ATOM	1675	NE	ARG	B	108	25.859	40.576	28.047	1.00	27.65
ATOM	1676	CZ	ARG	B	108	25.517	41.345	29.084	1.00	26.15
ATOM	1677	NH1	ARG	B	108	25.637	42.653	29.004	1.00	26.98
ATOM	1678	NH2	ARG	B	108	25.031	40.819	30.217	1.00	27.28
ATOM	1679	N	LEU	B	109	26.320	35.964	25.078	1.00	16.44
ATOM	1680	CA	LEU	B	109	25.649	34.700	25.242	1.00	19.58
ATOM	1681	C	LEU	B	109	24.667	34.827	26.384	1.00	19.57
ATOM	1682	O	LEU	B	109	24.963	35.423	27.418	1.00	21.90
ATOM	1683	CB	LEU	B	109	26.626	33.555	25.533	1.00	18.89
ATOM	1684	CG	LEU	B	109	27.661	33.129	24.491	1.00	20.14
ATOM	1685	CD1	LEU	B	109	28.673	32.188	25.119	1.00	18.71

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FIGURE 8A-39

ATOM	1686	CD2	LEU	B	109	26.985	32.436	23.316	1.00	22.74	C
ATOM	1687	N	PHE	B	110	23.477	34.293	26.119	1.00	19.30	N
ATOM	1688	CA	PHE	B	110	22.372	34.322	27.050	1.00	18.85	C
ATOM	1689	C	PHE	B	110	21.748	32.939	27.188	1.00	19.38	C
ATOM	1690	O	PHE	B	110	21.676	32.205	26.207	1.00	18.43	O
ATOM	1691	CB	PHE	B	110	21.312	35.298	26.553	1.00	17.38	C
ATOM	1692	CG	PHE	B	110	21.743	36.756	26.567	1.00	19.20	C
ATOM	1693	CD1	PHE	B	110	21.733	37.487	27.744	1.00	20.10	C
ATOM	1694	CD2	PHE	B	110	22.198	37.350	25.408	1.00	19.07	C
ATOM	1695	CE1	PHE	B	110	22.211	38.788	27.755	1.00	19.86	C
ATOM	1696	CE2	PHE	B	110	22.643	38.650	25.436	1.00	15.79	C
ATOM	1697	CZ	PHE	B	110	22.659	39.367	26.596	1.00	17.86	C
ATOM	1698	N	THR	B	111	21.246	32.547	28.376	1.00	18.40	N
ATOM	1699	CA	THR	B	111	20.431	31.336	28.505	1.00	14.95	C
ATOM	1700	C	THR	B	111	19.077	31.537	27.823	1.00	14.86	C
ATOM	1701	O	THR	B	111	18.720	32.705	27.696	1.00	18.62	O
ATOM	1702	CB	THR	B	111	20.254	30.986	30.016	1.00	10.83	C
ATOM	1703	OG1	THR	B	111	19.440	32.008	30.536	1.00	14.68	O
ATOM	1704	CG2	THR	B	111	21.520	31.006	30.845	1.00	11.33	C
ATOM	1705	N	PRO	B	112	18.205	30.602	27.418	1.00	14.14	N
ATOM	1706	CA	PRO	B	112	16.903	30.899	26.832	1.00	12.85	C
ATOM	1707	C	PRO	B	112	16.055	31.789	27.714	1.00	15.00	C
ATOM	1708	O	PRO	B	112	15.351	32.679	27.268	1.00	16.67	O
ATOM	1709	CB	PRO	B	112	16.297	29.536	26.730	1.00	13.18	C
ATOM	1710	CG	PRO	B	112	17.459	28.689	26.406	1.00	11.71	C
ATOM	1711	CD	PRO	B	112	18.482	29.179	27.402	1.00	12.63	C
ATOM	1712	N	GLU	B	113	16.103	31.597	29.015	1.00	17.42	N
ATOM	1713	CA	GLU	B	113	15.375	32.431	29.945	1.00	19.68	C
ATOM	1714	C	GLU	B	113	15.802	33.888	29.901	1.00	18.59	C
ATOM	1715	O	GLU	B	113	14.931	34.751	29.885	1.00	21.48	O
ATOM	1716	CB	GLU	B	113	15.546	31.841	31.328	1.00	22.92	C
ATOM	1717	CG	GLU	B	113	14.984	32.707	32.439	1.00	32.95	C
ATOM	1718	CD	GLU	B	113	15.763	32.704	33.770	1.00	39.93	C
ATOM	1719	OE1	GLU	B	113	16.869	33.281	33.900	1.00	41.39	O
ATOM	1720	OE2	GLU	B	113	15.193	32.144	34.712	1.00	44.90	O
ATOM	1721	N	GLU	B	114	17.096	34.210	29.885	1.00	18.49	N
ATOM	1722	CA	GLU	B	114	17.601	35.576	29.760	1.00	17.43	C
ATOM	1723	C	GLU	B	114	17.321	36.289	28.451	1.00	16.60	C
ATOM	1724	O	GLU	B	114	16.910	37.449	28.404	1.00	19.48	O
ATOM	1725	CB	GLU	B	114	19.090	35.543	29.980	1.00	19.55	C
ATOM	1726	CG	GLU	B	114	19.486	35.319	31.442	1.00	23.40	C
ATOM	1727	CD	GLU	B	114	20.962	35.034	31.718	1.00	25.98	C
ATOM	1728	OE1	GLU	B	114	21.730	34.826	30.765	1.00	25.41	O
ATOM	1729	OE2	GLU	B	114	21.322	34.982	32.906	1.00	28.77	O
ATOM	1730	N	PHE	B	115	17.507	35.551	27.379	1.00	14.86	N
ATOM	1731	CA	PHE	B	115	17.212	35.998	26.023	1.00	15.76	C
ATOM	1732	C	PHE	B	115	15.776	36.422	25.843	1.00	14.74	C
ATOM	1733	O	PHE	B	115	15.474	37.469	25.295	1.00	16.04	O
ATOM	1734	CB	PHE	B	115	17.513	34.865	25.012	1.00	14.37	C
ATOM	1735	CG	PHE	B	115	17.384	35.323	23.572	1.00	16.76	C
ATOM	1736	CD1	PHE	B	115	18.400	36.062	22.990	1.00	15.08	C
ATOM	1737	CD2	PHE	B	115	16.217	35.063	22.881	1.00	16.51	C
ATOM	1738	CE1	PHE	B	115	18.169	36.611	21.755	1.00	15.92	C
ATOM	1739	CE2	PHE	B	115	16.024	35.579	21.619	1.00	13.36	C
ATOM	1740	CZ	PHE	B	115	16.994	36.364	21.079	1.00	14.28	C
ATOM	1741	N	PHE	B	116	14.897	35.549	26.284	1.00	15.61	N
ATOM	1742	CA	PHE	B	116	13.497	35.810	26.150	1.00	15.94	C
ATOM	1743	C	PHE	B	116	12.918	36.798	27.125	1.00	16.92	C
ATOM	1744	O	PHE	B	116	11.842	37.326	26.862	1.00	18.97	O
ATOM	1745	CB	PHE	B	116	12.759	34.499	26.111	1.00	16.90	C

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FIGURE 8A-40

ATOM	1746	CG	PHE	B	116	12.962	33.796	24.776	1.00	16.87	C
ATOM	1747	CD1	PHE	B	116	12.315	34.278	23.639	1.00	16.00	C
ATOM	1748	CD2	PHE	B	116	13.830	32.714	24.689	1.00	17.13	C
ATOM	1749	CE1	PHE	B	116	12.558	33.654	22.429	1.00	17.64	C
ATOM	1750	CE2	PHE	B	116	14.079	32.114	23.482	1.00	16.31	C
ATOM	1751	CZ	PHE	B	116	13.427	32.582	22.349	1.00	17.77	C
ATOM	1752	N	ARG	B	117	13.629	37.094	28.208	1.00	17.01	N
ATOM	1753	CA	ARG	B	117	13.292	38.189	29.085	1.00	18.94	C
ATOM	1754	C	ARG	B	117	13.636	39.492	28.388	1.00	20.76	C
ATOM	1755	O	ARG	B	117	12.988	40.526	28.561	1.00	21.80	O
ATOM	1756	CB	ARG	B	117	14.124	38.043	30.361	1.00	22.28	C
ATOM	1757	CG	ARG	B	117	13.889	39.003	31.538	1.00	29.21	C
ATOM	1758	CD	ARG	B	117	13.292	38.359	32.834	1.00	35.23	C
ATOM	1759	NE	ARG	B	117	14.094	37.253	33.357	1.00	37.19	N
ATOM	1760	CZ	ARG	B	117	15.408	37.373	33.616	1.00	42.10	C
ATOM	1761	NH1	ARG	B	117	16.023	38.568	33.647	1.00	45.58	N
ATOM	1762	NH2	ARG	B	117	16.151	36.268	33.794	1.00	43.18	N
ATOM	1763	N	ILE	B	118	14.709	39.453	27.596	1.00	20.97	N
ATOM	1764	CA	ILE	B	118	15.078	40.588	26.807	1.00	18.77	C
ATOM	1765	C	ILE	B	118	14.103	40.799	25.662	1.00	20.54	C
ATOM	1766	O	ILE	B	118	13.592	41.896	25.487	1.00	20.49	O
ATOM	1767	CB	ILE	B	118	16.498	40.364	26.385	1.00	16.96	C
ATOM	1768	CG1	ILE	B	118	17.377	40.504	27.587	1.00	12.82	C
ATOM	1769	CG2	ILE	B	118	16.892	41.347	25.310	1.00	15.77	C
ATOM	1770	CD1	ILE	B	118	18.851	40.271	27.253	1.00	14.00	C
ATOM	1771	N	PHE	B	119	13.817	39.736	24.922	1.00	22.16	N
ATOM	1772	CA	PHE	B	119	12.840	39.717	23.864	1.00	23.96	C
ATOM	1773	C	PHE	B	119	11.528	40.271	24.356	1.00	26.51	C
ATOM	1774	O	PHE	B	119	10.934	41.093	23.674	1.00	29.24	O
ATOM	1775	CB	PHE	B	119	12.660	38.299	23.364	1.00	22.84	C
ATOM	1776	CG	PHE	B	119	11.555	38.173	22.327	1.00	24.88	C
ATOM	1777	CD1	PHE	B	119	11.811	38.512	21.006	1.00	25.69	C
ATOM	1778	CD2	PHE	B	119	10.271	37.803	22.727	1.00	24.94	C
ATOM	1779	CE1	PHE	B	119	10.748	38.539	20.122	1.00	25.07	C
ATOM	1780	CE2	PHE	B	119	9.216	37.831	21.844	1.00	24.69	C
ATOM	1781	CZ	PHE	B	119	9.465	38.212	20.539	1.00	25.22	C
ATOM	1782	N	ASN	B	120	11.076	39.898	25.540	1.00	29.22	N
ATOM	1783	CA	ASN	B	120	9.863	40.470	26.094	1.00	31.04	C
ATOM	1784	C	ASN	B	120	9.953	41.939	26.499	1.00	32.79	C
ATOM	1785	O	ASN	B	120	9.018	42.684	26.204	1.00	34.41	O
ATOM	1786	CB	ASN	B	120	9.343	39.640	27.253	1.00	29.44	C
ATOM	1787	CG	ASN	B	120	8.856	38.301	26.738	1.00	33.04	C
ATOM	1788	OD1	ASN	B	120	8.264	38.216	25.651	1.00	32.93	O
ATOM	1789	ND2	ASN	B	120	9.110	37.237	27.508	1.00	31.91	N
ATOM	1790	N	ARG	B	121	11.018	42.436	27.140	1.00	32.47	N
ATOM	1791	CA	ARG	B	121	11.117	43.849	27.465	1.00	30.92	C
ATOM	1792	C	ARG	B	121	11.067	44.709	26.204	1.00	29.78	C
ATOM	1793	O	ARG	B	121	10.444	45.760	26.207	1.00	28.95	O
ATOM	1794	CB	ARG	B	121	12.391	44.075	28.271	1.00	33.61	C
ATOM	1795	CG	ARG	B	121	12.655	45.523	28.664	1.00	41.90	C
ATOM	1796	CD	ARG	B	121	11.463	46.261	29.336	1.00	48.78	C
ATOM	1797	NE	ARG	B	121	11.048	47.453	28.567	1.00	55.93	N
ATOM	1798	CZ	ARG	B	121	11.568	48.694	28.762	1.00	59.13	C
ATOM	1799	NH1	ARG	B	121	12.543	48.894	29.659	1.00	60.86	N
ATOM	1800	NH2	ARG	B	121	11.124	49.767	28.074	1.00	60.62	N
ATOM	1801	N	SER	B	122	11.680	44.225	25.121	1.00	29.04	N
ATOM	1802	CA	SER	B	122	11.818	44.920	23.854	1.00	27.66	C
ATOM	1803	C	SER	B	122	10.512	45.006	23.126	1.00	29.01	C
ATOM	1804	O	SER	B	122	10.198	46.085	22.634	1.00	30.77	O
ATOM	1805	CB	SER	B	122	12.808	44.195	22.954	1.00	24.91	C

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FIGURE 8A-41

ATOM	1806	OG	SER	B	122	14.125	44.237	23.464	1.00	21.03	O
ATOM	1807	N	ILE	B	123	9.765	43.896	23.061	1.00	30.73	N
ATOM	1808	CA	ILE	B	123	8.427	43.886	22.488	1.00	33.96	C
ATOM	1809	C	ILE	B	123	7.513	44.857	23.232	1.00	38.09	C
ATOM	1810	O	ILE	B	123	6.743	45.579	22.610	1.00	38.61	O
ATOM	1811	CB	ILE	B	123	7.863	42.445	22.513	1.00	33.36	C
ATOM	1812	CG1	ILE	B	123	8.567	41.492	21.559	1.00	33.77	C
ATOM	1813	CG2	ILE	B	123	6.385	42.334	22.276	1.00	35.01	C
ATOM	1814	CD1	ILE	B	123	8.539	41.729	20.058	1.00	31.14	C
ATOM	1815	N	ASP	B	124	7.638	44.925	24.562	1.00	42.48	N
ATOM	1816	CA	ASP	B	124	6.868	45.809	25.424	1.00	45.69	C
ATOM	1817	C	ASP	B	124	7.347	47.237	25.404	1.00	45.68	C
ATOM	1818	O	ASP	B	124	6.592	48.118	25.836	1.00	46.88	O
ATOM	1819	CB	ASP	B	124	6.915	45.381	26.912	1.00	50.45	C
ATOM	1820	CG	ASP	B	124	6.483	43.950	27.274	1.00	56.00	C
ATOM	1821	OD1	ASP	B	124	5.766	43.310	26.481	1.00	61.21	O
ATOM	1822	OD2	ASP	B	124	6.883	43.461	28.344	1.00	56.72	O
ATOM	1823	N	ALA	B	125	8.599	47.461	24.970	1.00	46.60	N
ATOM	1824	CA	ALA	B	125	9.190	48.801	24.903	1.00	47.64	C
ATOM	1825	C	ALA	B	125	8.420	49.664	23.926	1.00	48.60	C
ATOM	1826	O	ALA	B	125	8.412	50.882	24.081	1.00	48.65	O
ATOM	1827	CB	ALA	B	125	10.643	48.781	24.422	1.00	46.01	C
ATOM	1828	N	PHE	B	126	7.752	49.014	22.960	1.00	50.56	N
ATOM	1829	CA	PHE	B	126	6.834	49.695	22.055	1.00	54.13	C
ATOM	1830	C	PHE	B	126	5.525	50.182	22.688	1.00	57.79	C
ATOM	1831	O	PHE	B	126	5.141	51.334	22.460	1.00	59.99	O
ATOM	1832	CB	PHE	B	126	6.538	48.850	20.810	1.00	51.52	C
ATOM	1833	CG	PHE	B	126	7.721	48.691	19.873	1.00	49.43	C
ATOM	1834	CD1	PHE	B	126	8.650	47.685	20.086	1.00	48.93	C
ATOM	1835	CD2	PHE	B	126	7.872	49.550	18.804	1.00	48.24	C
ATOM	1836	CE1	PHE	B	126	9.721	47.531	19.226	1.00	47.28	C
ATOM	1837	CE2	PHE	B	126	8.960	49.402	17.969	1.00	46.11	C
ATOM	1838	CZ	PHE	B	126	9.882	48.401	18.174	1.00	45.91	C
ATOM	1839	N	LYS	B	127	4.843	49.346	23.505	1.00	61.28	N
ATOM	1840	CA	LYS	B	127	3.558	49.636	24.178	1.00	62.20	C
ATOM	1841	C	LYS	B	127	3.454	50.906	25.026	1.00	62.03	C
ATOM	1842	O	LYS	B	127	2.394	51.539	25.092	1.00	61.71	O
ATOM	1843	CB	LYS	B	127	3.115	48.458	25.090	1.00	64.81	C
ATOM	1844	CG	LYS	B	127	2.463	47.185	24.502	1.00	65.92	C
ATOM	1845	CD	LYS	B	127	2.082	46.311	25.702	1.00	67.81	C
ATOM	1846	CE	LYS	B	127	2.369	44.834	25.433	1.00	69.44	C
ATOM	1847	NZ	LYS	B	127	2.594	44.129	26.691	1.00	68.14	N
ATOM	1848	N	ASP	B	128	4.561	51.200	25.719	1.00	62.76	N
ATOM	1849	CA	ASP	B	128	4.736	52.380	26.554	1.00	62.70	C
ATOM	1850	C	ASP	B	128	5.573	53.412	25.794	1.00	63.56	C
ATOM	1851	O	ASP	B	128	6.638	53.838	26.251	1.00	64.23	O
ATOM	1852	CB	ASP	B	128	5.480	51.925	27.833	1.00	62.32	C
ATOM	1853	N	PHE	B	129	5.128	53.802	24.587	1.00	64.47	N
ATOM	1854	CA	PHE	B	129	5.813	54.828	23.801	1.00	65.58	C
ATOM	1855	C	PHE	B	129	5.172	56.224	23.900	1.00	66.25	C
ATOM	1856	O	PHE	B	129	4.145	56.473	23.258	1.00	67.17	O
ATOM	1857	CB	PHE	B	129	5.971	54.368	22.338	1.00	64.56	C
ATOM	1858	CG	PHE	B	129	7.424	54.230	21.907	1.00	63.61	C
ATOM	1859	CD1	PHE	B	129	8.187	55.356	21.634	1.00	64.45	C
ATOM	1860	CD2	PHE	B	129	7.979	52.977	21.775	1.00	62.93	C
ATOM	1861	CE1	PHE	B	129	9.503	55.219	21.235	1.00	64.07	C
ATOM	1862	CE2	PHE	B	129	9.291	52.837	21.378	1.00	63.56	C
ATOM	1863	CZ	PHE	B	129	10.048	53.959	21.111	1.00	64.70	C
ATOM	1864	N	ASP	B	137	17.272	62.584	24.623	1.00	55.18	N
ATOM	1865	CA	ASP	B	137	18.560	63.025	24.106	1.00	54.96	C

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FIGURE 8A-42

ATOM	1866	C	ASP	B	137	19.597	61.931	23.769	1.00	55.95	C
ATOM	1867	O	ASP	B	137	20.291	62.026	22.743	1.00	55.11	O
ATOM	1868	CB	ASP	B	137	19.180	63.952	25.136	1.00	53.99	C
ATOM	1869	N	CYS	B	138	19.669	60.900	24.656	1.00	55.99	N
ATOM	1870	CA	CYS	B	138	20.594	59.741	24.665	1.00	55.50	C
ATOM	1871	C	CYS	B	138	22.065	59.964	25.031	1.00	55.10	C
ATOM	1872	O	CYS	B	138	22.723	58.973	25.357	1.00	55.77	O
ATOM	1873	CB	CYS	B	138	20.486	58.822	23.416	1.00	53.55	C
ATOM	1874	SG	CYS	B	138	18.766	58.362	23.058	1.00	53.01	S
TER	1876		CYS	B	138						
ATOM	1877	N	ASN	C	11	51.574	13.978	45.345	1.00	51.40	N
ATOM	1878	CA	ASN	C	11	50.150	14.075	45.169	1.00	50.61	C
ATOM	1879	C	ASN	C	11	49.636	15.080	46.231	1.00	51.75	C
ATOM	1880	O	ASN	C	11	49.446	16.244	45.828	1.00	52.28	O
ATOM	1881	CB	ASN	C	11	49.486	12.671	45.271	1.00	48.14	C
ATOM	1882	N	VAL	C	12	49.577	14.664	47.548	1.00	49.74	N
ATOM	1883	CA	VAL	C	12	48.941	15.269	48.771	1.00	46.17	C
ATOM	1884	C	VAL	C	12	49.317	16.681	49.255	1.00	43.47	C
ATOM	1885	O	VAL	C	12	48.526	17.397	49.868	1.00	42.02	O
ATOM	1886	CB	VAL	C	12	49.032	14.271	50.044	1.00	47.02	C
ATOM	1887	CG1	VAL	C	12	50.479	14.042	50.561	1.00	46.01	C
ATOM	1888	CG2	VAL	C	12	48.129	14.662	51.233	1.00	44.78	C
ATOM	1889	N	LYS	C	13	50.588	17.052	49.054	1.00	43.09	N
ATOM	1890	CA	LYS	C	13	51.082	18.424	49.218	1.00	39.49	C
ATOM	1891	C	LYS	C	13	50.370	19.321	48.180	1.00	36.49	C
ATOM	1892	O	LYS	C	13	49.910	20.435	48.472	1.00	35.14	O
ATOM	1893	CB	LYS	C	13	52.643	18.424	48.986	1.00	37.77	C
ATOM	1894	N	ASP	C	14	50.231	18.776	46.951	1.00	33.25	N
ATOM	1895	CA	ASP	C	14	49.522	19.456	45.898	1.00	27.29	C
ATOM	1896	C	ASP	C	14	48.042	19.262	45.991	1.00	21.51	C
ATOM	1897	O	ASP	C	14	47.408	20.205	45.602	1.00	20.53	O
ATOM	1898	CB	ASP	C	14	50.101	19.142	44.565	1.00	31.10	C
ATOM	1899	CG	ASP	C	14	51.439	19.856	44.288	1.00	35.88	C
ATOM	1900	OD1	ASP	C	14	52.043	20.514	45.155	1.00	37.80	O
ATOM	1901	OD2	ASP	C	14	51.890	19.755	43.143	1.00	37.19	O
ATOM	1902	N	VAL	C	15	47.447	18.202	46.526	1.00	15.89	N
ATOM	1903	CA	VAL	C	15	46.073	18.270	46.962	1.00	16.75	C
ATOM	1904	C	VAL	C	15	45.796	19.433	47.938	1.00	17.73	C
ATOM	1905	O	VAL	C	15	44.821	20.167	47.775	1.00	18.15	O
ATOM	1906	CB	VAL	C	15	45.653	16.905	47.548	1.00	17.03	C
ATOM	1907	CG1	VAL	C	15	44.266	16.920	48.161	1.00	15.16	C
ATOM	1908	CG2	VAL	C	15	45.656	15.889	46.430	1.00	17.49	C
ATOM	1909	N	THR	C	16	46.659	19.692	48.910	1.00	17.16	N
ATOM	1910	CA	THR	C	16	46.513	20.824	49.806	1.00	16.51	C
ATOM	1911	C	THR	C	16	46.660	22.151	49.096	1.00	15.07	C
ATOM	1912	O	THR	C	16	45.901	23.049	49.418	1.00	16.99	O
ATOM	1913	CB	THR	C	16	47.533	20.674	51.000	1.00	17.35	C
ATOM	1914	OG1	THR	C	16	47.059	19.546	51.734	1.00	19.10	O
ATOM	1915	CG2	THR	C	16	47.615	21.868	51.934	1.00	11.74	C
ATOM	1916	N	LYS	C	17	47.562	22.381	48.160	1.00	13.81	N
ATOM	1917	CA	LYS	C	17	47.496	23.602	47.390	1.00	15.88	C
ATOM	1918	C	LYS	C	17	46.197	23.789	46.541	1.00	16.97	C
ATOM	1919	O	LYS	C	17	45.608	24.877	46.465	1.00	17.88	O
ATOM	1920	CB	LYS	C	17	48.702	23.598	46.505	1.00	18.13	C
ATOM	1921	CG	LYS	C	17	50.006	23.615	47.257	1.00	21.24	C
ATOM	1922	CD	LYS	C	17	51.103	23.441	46.198	1.00	24.88	C
ATOM	1923	CE	LYS	C	17	52.486	23.537	46.798	1.00	28.59	C
ATOM	1924	NZ	LYS	C	17	52.730	24.883	47.284	1.00	31.31	N
ATOM	1925	N	LEU	C	18	45.682	22.736	45.880	1.00	14.39	N
ATOM	1926	CA	LEU	C	18	44.454	22.764	45.149	1.00	11.22	C

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FIGURE 8A-43

ATOM	1927	C	LEU	C	18	43.333	23.111	46.047	1.00	10.78	C
ATOM	1928	O	LEU	C	18	42.612	24.032	45.691	1.00	16.08	O
ATOM	1929	CB	LEU	C	18	44.129	21.412	44.609	1.00	12.69	C
ATOM	1930	CG	LEU	C	18	42.973	21.312	43.632	1.00	15.70	C
ATOM	1931	CD1	LEU	C	18	43.151	22.220	42.429	1.00	9.04	C
ATOM	1932	CD2	LEU	C	18	42.864	19.875	43.248	1.00	15.11	N
ATOM	1933	N	VAL	C	19	43.155	22.484	47.210	1.00	11.81	C
ATOM	1934	CA	VAL	C	19	42.092	22.868	48.138	1.00	12.12	C
ATOM	1935	C	VAL	C	19	42.159	24.359	48.569	1.00	13.12	O
ATOM	1936	O	VAL	C	19	41.144	25.056	48.607	1.00	14.59	C
ATOM	1937	CB	VAL	C	19	42.041	21.868	49.328	1.00	12.63	C
ATOM	1938	CG1	VAL	C	19	40.984	22.267	50.328	1.00	11.49	C
ATOM	1939	CG2	VAL	C	19	41.661	20.496	48.835	1.00	12.48	N
ATOM	1940	N	ALA	C	20	43.362	24.909	48.821	1.00	13.02	C
ATOM	1941	CA	ALA	C	20	43.532	26.278	49.252	1.00	11.77	C
ATOM	1942	C	ALA	C	20	43.254	27.224	48.126	1.00	11.25	O
ATOM	1943	O	ALA	C	20	42.888	28.357	48.344	1.00	14.74	C
ATOM	1944	CB	ALA	C	20	44.975	26.452	49.635	1.00	10.68	C
ATOM	1945	N	ASN	C	21	43.461	26.757	46.895	1.00	15.11	N
ATOM	1946	CA	ASN	C	21	43.197	27.471	45.648	1.00	13.34	C
ATOM	1947	C	ASN	C	21	41.898	27.107	44.949	1.00	13.09	C
ATOM	1948	O	ASN	C	21	41.663	27.533	43.815	1.00	18.62	O
ATOM	1949	CB	ASN	C	21	44.318	27.149	44.717	1.00	12.84	C
ATOM	1950	CG	ASN	C	21	45.401	28.151	44.755	1.00	12.42	C
ATOM	1951	OD1	ASN	C	21	45.277	29.229	45.315	1.00	14.66	O
ATOM	1952	ND2	ASN	C	21	46.503	27.827	44.131	1.00	12.99	N
ATOM	1953	N	LEU	C	22	41.041	26.311	45.536	1.00	12.25	N
ATOM	1954	CA	LEU	C	22	39.691	26.194	45.063	1.00	12.28	C
ATOM	1955	C	LEU	C	22	38.831	27.012	45.972	1.00	12.85	O
ATOM	1956	O	LEU	C	22	39.216	27.109	47.126	1.00	17.11	C
ATOM	1957	CB	LEU	C	22	39.202	24.755	45.039	1.00	10.06	C
ATOM	1958	CG	LEU	C	22	39.745	23.906	43.936	1.00	9.08	C
ATOM	1959	CD1	LEU	C	22	39.380	22.464	44.120	1.00	8.06	C
ATOM	1960	CD2	LEU	C	22	39.124	24.394	42.666	1.00	11.26	N
ATOM	1961	N	PRO	C	23	37.706	27.649	45.629	1.00	12.49	C
ATOM	1962	CA	PRO	C	23	36.902	28.384	46.592	1.00	12.26	C
ATOM	1963	C	PRO	C	23	36.214	27.457	47.604	1.00	13.42	O
ATOM	1964	O	PRO	C	23	35.695	26.416	47.220	1.00	13.22	C
ATOM	1965	CB	PRO	C	23	35.923	29.108	45.681	1.00	13.14	C
ATOM	1966	CG	PRO	C	23	36.407	29.009	44.237	1.00	9.94	C
ATOM	1967	CD	PRO	C	23	37.094	27.667	44.292	1.00	12.73	N
ATOM	1968	N	LYS	C	24	36.216	27.796	48.898	1.00	13.54	C
ATOM	1969	CA	LYS	C	24	35.515	27.039	49.919	1.00	17.03	C
ATOM	1970	C	LYS	C	24	34.053	26.703	49.596	1.00	17.41	O
ATOM	1971	O	LYS	C	24	33.500	25.693	50.011	1.00	15.96	C
ATOM	1972	CB	LYS	C	24	35.591	27.845	51.228	1.00	17.76	C
ATOM	1973	CG	LYS	C	24	36.918	27.585	51.896	1.00	22.90	C
ATOM	1974	CD	LYS	C	24	37.423	28.782	52.700	1.00	24.73	C
ATOM	1975	CE	LYS	C	24	38.893	28.608	53.191	1.00	25.32	N
ATOM	1976	NZ	LYS	C	24	39.427	29.914	53.578	1.00	27.67	N
ATOM	1977	N	ASP	C	25	33.380	27.526	48.807	1.00	20.45	C
ATOM	1978	CA	ASP	C	25	31.969	27.349	48.579	1.00	20.93	C
ATOM	1979	C	ASP	C	25	31.690	26.924	47.164	1.00	19.35	O
ATOM	1980	O	ASP	C	25	30.617	27.146	46.603	1.00	21.38	C
ATOM	1981	CB	ASP	C	25	31.316	28.665	48.909	1.00	23.07	C
ATOM	1982	CG	ASP	C	25	31.726	29.820	48.014	1.00	28.48	O
ATOM	1983	OD1	ASP	C	25	32.736	29.755	47.329	1.00	29.48	O
ATOM	1984	OD2	ASP	C	25	31.018	30.829	48.006	1.00	35.37	N
ATOM	1985	N	TYR	C	26	32.684	26.330	46.570	1.00	17.08	C
ATOM	1986	CA	TYR	C	26	32.486	25.784	45.270	1.00	18.09	

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FIGURE 8A-44

ATOM	1987	C	TYR	C	26	32.066	24.352	45.473	1.00	20.16
ATOM	1988	O	TYR	C	26	32.672	23.586	46.210	1.00	20.74
ATOM	1989	CB	TYR	C	26	33.787	25.925	44.505	1.00	18.65
ATOM	1990	CG	TYR	C	26	33.779	25.389	43.087	1.00	15.43
ATOM	1991	CD1	TYR	C	26	32.863	25.870	42.180	1.00	14.28
ATOM	1992	CD2	TYR	C	26	34.687	24.394	42.740	1.00	18.66
ATOM	1993	CE1	TYR	C	26	32.828	25.305	40.916	1.00	18.89
ATOM	1994	CE2	TYR	C	26	34.680	23.853	41.457	1.00	18.57
ATOM	1995	CZ	TYR	C	26	33.736	24.325	40.567	1.00	17.94
ATOM	1996	OH	TYR	C	26	33.702	23.844	39.293	1.00	20.05
HETATM	1997	N	MSE	C	27	30.992	23.977	44.806	1.00	22.38
HETATM	1998	CA	MSE	C	27	30.472	22.643	44.960	1.00	23.82
HETATM	1999	C	MSE	C	27	30.902	21.790	43.796	1.00	23.07
HETATM	2000	O	MSE	C	27	30.675	22.180	42.659	1.00	22.78
HETATM	2001	CB	MSE	C	27	28.966	22.685	45.023	1.00	27.76
HETATM	2002	CG	MSE	C	27	28.476	23.440	46.222	1.00	33.28
HETATM	2003	SE	MSE	C	27	29.250	22.864	47.919	1.00	47.63
HETATM	2004	CE	MSE	C	27	28.807	24.413	48.975	1.00	42.81
ATOM	2005	N	ILE	C	28	31.514	20.637	44.127	1.00	23.36
ATOM	2006	CA	ILE	C	28	31.890	19.552	43.196	1.00	24.49
ATOM	2007	C	ILE	C	28	30.924	18.334	43.195	1.00	25.21
ATOM	2008	O	ILE	C	28	30.568	17.795	44.237	1.00	24.49
ATOM	2009	CB	ILE	C	28	33.364	19.075	43.497	1.00	21.68
ATOM	2010	CG1	ILE	C	28	34.379	20.215	43.453	1.00	19.99
ATOM	2011	CG2	ILE	C	28	33.796	18.049	42.485	1.00	19.57
ATOM	2012	CD1	ILE	C	28	35.761	19.859	43.991	1.00	18.85
ATOM	2013	N	THR	C	29	30.508	17.846	42.017	1.00	26.46
ATOM	2014	CA	THR	C	29	29.637	16.688	41.888	1.00	26.80
ATOM	2015	C	THR	C	29	30.388	15.361	41.957	1.00	27.21
ATOM	2016	O	THR	C	29	31.299	15.084	41.182	1.00	26.27
ATOM	2017	CB	THR	C	29	28.824	16.736	40.580	1.00	25.22
ATOM	2018	OG1	THR	C	29	28.137	17.962	40.566	1.00	28.05
ATOM	2019	CG2	THR	C	29	27.773	15.659	40.545	1.00	26.26
ATOM	2020	N	LEU	C	30	29.980	14.498	42.878	1.00	27.91
ATOM	2021	CA	LEU	C	30	30.519	13.157	42.943	1.00	29.69
ATOM	2022	C	LEU	C	30	29.354	12.189	43.168	1.00	31.34
ATOM	2023	O	LEU	C	30	28.542	12.362	44.080	1.00	30.99
ATOM	2024	CB	LEU	C	30	31.578	13.070	44.051	1.00	25.27
ATOM	2025	CG	LEU	C	30	32.157	11.727	44.434	1.00	23.15
ATOM	2026	CD1	LEU	C	30	32.879	11.106	43.274	1.00	22.85
ATOM	2027	CD2	LEU	C	30	33.110	11.943	45.570	1.00	25.04
ATOM	2028	N	LYS	C	31	29.246	11.172	42.300	1.00	34.65
ATOM	2029	CA	LYS	C	31	28.335	10.045	42.513	1.00	36.49
ATOM	2030	C	LYS	C	31	28.910	9.150	43.620	1.00	36.03
ATOM	2031	O	LYS	C	31	29.741	8.287	43.370	1.00	36.42
ATOM	2032	CB	LYS	C	31	28.121	9.241	41.218	1.00	36.56
ATOM	2033	CG	LYS	C	31	27.475	9.966	40.056	1.00	39.42
ATOM	2034	CD	LYS	C	31	26.867	8.902	39.121	1.00	47.68
ATOM	2035	CE	LYS	C	31	25.930	9.427	37.990	1.00	51.31
ATOM	2036	NZ	LYS	C	31	24.859	8.496	37.602	1.00	51.86
ATOM	2037	N	TYR	C	32	28.514	9.411	44.868	1.00	38.89
ATOM	2038	CA	TYR	C	32	29.122	8.846	46.061	1.00	40.86
ATOM	2039	C	TYR	C	32	28.594	7.437	46.265	1.00	43.51
ATOM	2040	O	TYR	C	32	27.425	7.204	45.953	1.00	45.02
ATOM	2041	CB	TYR	C	32	28.707	9.747	47.229	1.00	37.67
ATOM	2042	CG	TYR	C	32	29.138	9.317	48.610	1.00	41.48
ATOM	2043	CD1	TYR	C	32	30.459	9.438	48.984	1.00	43.11
ATOM	2044	CD2	TYR	C	32	28.190	8.877	49.536	1.00	43.18
ATOM	2045	CE1	TYR	C	32	30.812	9.172	50.302	1.00	44.55
ATOM	2046	CE2	TYR	C	32	28.542	8.584	50.847	1.00	44.09

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FIGURE 8A-45

ATOM	2047	CZ	TYR	C	32	29.862	8.758	51.230	1.00	45.88
ATOM	2048	OH	TYR	C	32	30.238	8.549	52.557	1.00	49.38
ATOM	2049	N	VAL	C	33	29.391	6.459	46.718	1.00	46.10
ATOM	2050	CA	VAL	C	33	28.866	5.097	46.885	1.00	48.63
ATOM	2051	C	VAL	C	33	28.323	4.935	48.307	1.00	50.48
ATOM	2052	O	VAL	C	33	29.088	5.086	49.265	1.00	49.75
ATOM	2053	CB	VAL	C	33	29.900	4.000	46.501	1.00	49.02
ATOM	2054	CG1	VAL	C	33	29.390	2.594	46.823	1.00	50.53
ATOM	2055	CG2	VAL	C	33	30.216	4.072	45.014	1.00	47.63
ATOM	2056	N	PRO	C	34	27.006	4.682	48.505	1.00	53.28
ATOM	2057	CA	PRO	C	34	26.385	4.695	49.834	1.00	55.66
ATOM	2058	C	PRO	C	34	27.121	3.734	50.767	1.00	58.89
ATOM	2059	O	PRO	C	34	27.426	2.568	50.448	1.00	59.22
ATOM	2060	CB	PRO	C	34	24.936	4.297	49.549	1.00	54.96
ATOM	2061	CG	PRO	C	34	24.701	4.825	48.139	1.00	51.80
ATOM	2062	CD	PRO	C	34	26.002	4.428	47.456	1.00	51.86
ATOM	2063	N	GLY	C	35	27.545	4.399	51.850	1.00	60.51
ATOM	2064	CA	GLY	C	35	28.272	3.744	52.925	1.00	62.88
ATOM	2065	C	GLY	C	35	29.632	3.266	52.457	1.00	63.14
ATOM	2066	O	GLY	C	35	29.852	2.077	52.214	1.00	64.01
HETATM	2067	N	MSE	C	36	30.521	4.240	52.301	1.00	62.92
HETATM	2068	CA	MSE	C	36	31.881	3.970	51.881	1.00	63.09
HETATM	2069	C	MSE	C	36	32.945	4.485	52.836	1.00	64.77
HETATM	2070	O	MSE	C	36	34.148	4.357	52.599	1.00	65.03
HETATM	2071	CB	MSE	C	36	32.115	4.582	50.531	1.00	62.61
HETATM	2072	CG	MSE	C	36	31.973	6.068	50.551	1.00	60.55
HETATM	2073	SE	MSE	C	36	33.277	6.879	49.401	1.00	61.18
HETATM	2074	CE	MSE	C	36	34.541	7.346	50.777	1.00	55.15
ATOM	2075	N	ASP	C	37	32.430	5.163	53.863	1.00	66.73
ATOM	2076	CA	ASP	C	37	33.149	5.583	55.061	1.00	67.41
ATOM	2077	C	ASP	C	37	33.215	4.481	56.132	1.00	66.85
ATOM	2078	O	ASP	C	37	34.130	4.393	56.957	1.00	67.21
ATOM	2079	CB	ASP	C	37	32.478	6.867	55.589	1.00	69.00
ATOM	2080	CG	ASP	C	37	30.982	6.808	55.935	1.00	70.25
ATOM	2081	OD1	ASP	C	37	30.143	6.538	55.061	1.00	69.81
ATOM	2082	OD2	ASP	C	37	30.657	7.058	57.097	1.00	71.69
ATOM	2083	N	VAL	C	38	32.224	3.593	56.068	1.00	65.94
ATOM	2084	CA	VAL	C	38	32.091	2.461	56.960	1.00	64.55
ATOM	2085	C	VAL	C	38	32.395	1.200	56.170	1.00	65.94
ATOM	2086	O	VAL	C	38	33.340	0.521	56.584	1.00	68.33
ATOM	2087	CB	VAL	C	38	30.694	2.475	57.631	1.00	63.05
ATOM	2088	CG1	VAL	C	38	29.960	1.135	57.787	1.00	62.73
ATOM	2089	CG2	VAL	C	38	30.915	3.097	58.990	1.00	61.39
ATOM	2090	N	LEU	C	39	31.700	0.861	55.059	1.00	64.32
ATOM	2091	CA	LEU	C	39	31.997	-0.365	54.328	1.00	63.23
ATOM	2092	C	LEU	C	39	33.487	-0.412	53.952	1.00	62.57
ATOM	2093	O	LEU	C	39	34.084	0.647	53.713	1.00	63.24
ATOM	2094	CB	LEU	C	39	31.130	-0.449	53.078	1.00	62.74
ATOM	2095	N	PRO	C	40	34.161	-1.578	54.006	1.00	61.57
ATOM	2096	CA	PRO	C	40	35.608	-1.719	53.761	1.00	59.74
ATOM	2097	C	PRO	C	40	36.009	-1.462	52.318	1.00	57.52
ATOM	2098	O	PRO	C	40	35.183	-1.629	51.418	1.00	54.10
ATOM	2099	CB	PRO	C	40	35.861	-3.170	54.123	1.00	60.55
ATOM	2100	CG	PRO	C	40	34.550	-3.863	53.762	1.00	60.74
ATOM	2101	CD	PRO	C	40	33.546	-2.868	54.329	1.00	61.16
ATOM	2102	N	SER	C	41	37.282	-1.110	52.111	1.00	56.39
ATOM	2103	CA	SER	C	41	37.779	-0.735	50.798	1.00	56.77
ATOM	2104	C	SER	C	41	37.271	-1.553	49.602	1.00	56.41
ATOM	2105	O	SER	C	41	36.627	-0.992	48.727	1.00	56.58
ATOM	2106	CB	SER	C	41	39.292	-0.643	50.831	1.00	57.36

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FIGURE 8A-46

ATOM	2107	OG	SER	C	41	39.964	-1.877	50.695	1.00	60.69	O
ATOM	2108	N	HIS	C	42	37.404	-2.882	49.580	1.00	56.11	N
ATOM	2109	CA	HIS	C	42	36.947	-3.739	48.482	1.00	56.80	C
ATOM	2110	C	HIS	C	42	35.473	-3.664	48.079	1.00	56.34	C
ATOM	2111	O	HIS	C	42	35.062	-4.139	47.007	1.00	55.64	O
ATOM	2112	CB	HIS	C	42	37.301	-5.217	48.795	1.00	60.78	C
ATOM	2113	CG	HIS	C	42	36.205	-6.095	49.445	1.00	63.24	C
ATOM	2114	ND1	HIS	C	42	35.894	-6.211	50.736	1.00	63.50	N
ATOM	2115	CD2	HIS	C	42	35.244	-6.788	48.711	1.00	63.78	C
ATOM	2116	CE1	HIS	C	42	34.762	-6.882	50.802	1.00	64.65	C
ATOM	2117	NE2	HIS	C	42	34.371	-7.201	49.584	1.00	64.49	N
ATOM	2118	N	CYS	C	43	34.669	-3.175	49.027	1.00	56.27	N
ATOM	2119	CA	CYS	C	43	33.239	-3.012	48.806	1.00	56.25	C
ATOM	2120	C	CYS	C	43	32.953	-1.871	47.844	1.00	54.69	C
ATOM	2121	O	CYS	C	43	32.104	-2.006	46.959	1.00	56.17	O
ATOM	2122	CB	CYS	C	43	32.488	-2.787	50.120	1.00	57.47	C
ATOM	2123	SG	CYS	C	43	31.647	-4.253	50.786	1.00	60.51	S
ATOM	2124	N	TRP	C	44	33.695	-0.766	47.973	1.00	51.41	N
ATOM	2125	CA	TRP	C	44	33.338	0.464	47.287	1.00	47.58	C
ATOM	2126	C	TRP	C	44	34.349	0.946	46.300	1.00	46.08	C
ATOM	2127	O	TRP	C	44	33.969	1.593	45.341	1.00	46.29	O
ATOM	2128	CB	TRP	C	44	33.089	1.587	48.271	1.00	47.09	C
ATOM	2129	CG	TRP	C	44	34.199	1.801	49.301	1.00	46.63	C
ATOM	2130	CD1	TRP	C	44	34.221	1.046	50.444	1.00	47.77	C
ATOM	2131	CD2	TRP	C	44	35.261	2.660	49.225	1.00	45.55	C
ATOM	2132	NE1	TRP	C	44	35.307	1.419	51.078	1.00	47.46	N
ATOM	2133	CE2	TRP	C	44	35.948	2.361	50.389	1.00	44.86	C
ATOM	2134	CE3	TRP	C	44	35.723	3.640	48.403	1.00	42.70	C
ATOM	2135	CZ2	TRP	C	44	37.122	2.956	50.754	1.00	43.79	C
ATOM	2136	CZ3	TRP	C	44	36.886	4.263	48.782	1.00	43.82	C
ATOM	2137	CH2	TRP	C	44	37.597	3.925	49.920	1.00	42.91	C
ATOM	2138	N	ILE	C	45	35.615	0.635	46.539	1.00	45.14	N
ATOM	2139	CA	ILE	C	45	36.735	1.252	45.851	1.00	47.08	C
ATOM	2140	C	ILE	C	45	36.657	1.198	44.329	1.00	47.61	C
ATOM	2141	O	ILE	C	45	36.955	2.157	43.619	1.00	48.87	O
ATOM	2142	CB	ILE	C	45	38.085	0.681	46.427	1.00	47.91	C
ATOM	2143	CG1	ILE	C	45	39.316	1.515	46.123	1.00	46.35	C
ATOM	2144	CG2	ILE	C	45	38.420	-0.723	45.905	1.00	50.05	C
ATOM	2145	CD1	ILE	C	45	39.180	2.995	46.462	1.00	43.72	C
ATOM	2146	N	SER	C	46	36.158	0.077	43.850	1.00	47.61	N
ATOM	2147	CA	SER	C	46	36.069	-0.245	42.437	1.00	48.09	C
ATOM	2148	C	SER	C	46	35.166	0.685	41.595	1.00	47.26	C
ATOM	2149	O	SER	C	46	35.598	1.186	40.555	1.00	46.49	O
ATOM	2150	CB	SER	C	46	35.688	-1.728	42.427	1.00	50.90	C
ATOM	2151	OG	SER	C	46	35.093	-2.219	43.664	1.00	54.24	O
ATOM	2152	N	GLU	C	47	33.932	0.997	42.039	1.00	46.80	N
ATOM	2153	CA	GLU	C	47	33.095	2.037	41.430	1.00	45.94	C
ATOM	2154	C	GLU	C	47	33.599	3.449	41.776	1.00	43.82	C
ATOM	2155	O	GLU	C	47	33.532	4.348	40.947	1.00	43.16	O
ATOM	2156	CB	GLU	C	47	31.602	1.843	41.831	1.00	47.29	C
ATOM	2157	CG	GLU	C	47	30.478	2.752	41.246	1.00	52.00	C
ATOM	2158	CD	GLU	C	47	29.748	2.394	39.936	1.00	54.16	C
ATOM	2159	OE1	GLU	C	47	28.894	1.494	39.926	1.00	57.21	O
ATOM	2160	OE2	GLU	C	47	29.989	3.052	38.922	1.00	54.36	O
HETATM	2161	N	MSE	C	48	34.170	3.670	42.967	1.00	43.01	N
HETATM	2162	CA	MSE	C	48	34.601	4.979	43.448	1.00	40.77	C
HETATM	2163	C	MSE	C	48	35.795	5.538	42.724	1.00	37.10	C
HETATM	2164	O	MSE	C	48	35.799	6.739	42.563	1.00	39.16	O
HETATM	2165	CB	MSE	C	48	34.926	4.968	44.927	1.00	43.83	C
HETATM	2166	CG	MSE	C	48	34.667	6.334	45.551	1.00	49.60	C

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FIGURE 8A-47

HETATM	2167	SE	MSE	C	48	32.809	6.850	45.340	1.00	57.46	SE
HETATM	2168	CE	MSE	C	48	32.917	8.464	46.266	1.00	52.90	C
ATOM	2169	N	VAL	C	49	36.793	4.773	42.266	1.00	34.29	N
ATOM	2170	CA	VAL	C	49	37.855	5.271	41.388	1.00	30.22	C
ATOM	2171	C	VAL	C	49	37.372	5.680	39.997	1.00	31.03	C
ATOM	2172	O	VAL	C	49	37.936	6.572	39.365	1.00	30.17	O
ATOM	2173	CB	VAL	C	49	39.021	4.288	41.268	1.00	27.65	C
ATOM	2174	CG1	VAL	C	49	39.719	4.131	42.581	1.00	27.80	C
ATOM	2175	CG2	VAL	C	49	38.591	2.924	40.828	1.00	27.38	C
ATOM	2176	N	VAL	C	50	36.319	5.056	39.478	1.00	29.68	N
ATOM	2177	CA	VAL	C	50	35.727	5.548	38.255	1.00	29.53	C
ATOM	2178	C	VAL	C	50	34.932	6.806	38.559	1.00	28.57	C
ATOM	2179	O	VAL	C	50	35.069	7.755	37.800	1.00	30.41	O
ATOM	2180	CB	VAL	C	50	34.904	4.446	37.554	1.00	30.06	C
ATOM	2181	CG1	VAL	C	50	34.026	4.900	36.371	1.00	28.50	C
ATOM	2182	CG2	VAL	C	50	35.916	3.457	37.070	1.00	29.52	C
ATOM	2183	N	GLN	C	51	34.147	6.917	39.639	1.00	28.05	N
ATOM	2184	CA	GLN	C	51	33.421	8.148	39.945	1.00	27.55	C
ATOM	2185	C	GLN	C	51	34.267	9.336	40.379	1.00	26.77	C
ATOM	2186	O	GLN	C	51	33.957	10.480	40.061	1.00	27.78	O
ATOM	2187	CB	GLN	C	51	32.276	7.962	40.944	1.00	27.95	C
ATOM	2188	CG	GLN	C	51	31.142	7.029	40.503	1.00	31.66	C
ATOM	2189	CD	GLN	C	51	30.518	7.274	39.121	1.00	35.14	C
ATOM	2190	OE1	GLN	C	51	30.531	8.353	38.510	1.00	34.94	O
ATOM	2191	NE2	GLN	C	51	29.945	6.214	38.566	1.00	36.11	N
ATOM	2192	N	LEU	C	52	35.349	9.130	41.113	1.00	24.84	N
ATOM	2193	CA	LEU	C	52	36.290	10.188	41.316	1.00	24.73	C
ATOM	2194	C	LEU	C	52	36.914	10.560	40.004	1.00	25.82	C
ATOM	2195	O	LEU	C	52	37.061	11.752	39.750	1.00	26.91	O
ATOM	2196	CB	LEU	C	52	37.349	9.754	42.251	1.00	25.92	C
ATOM	2197	CG	LEU	C	52	36.831	9.701	43.653	1.00	27.26	C
ATOM	2198	CD1	LEU	C	52	37.880	9.090	44.510	1.00	27.86	C
ATOM	2199	CD2	LEU	C	52	36.473	11.078	44.141	1.00	27.93	C
ATOM	2200	N	SER	C	53	37.211	9.566	39.148	1.00	27.18	N
ATOM	2201	CA	SER	C	53	37.788	9.790	37.838	1.00	24.69	C
ATOM	2202	C	SER	C	53	36.859	10.558	36.918	1.00	26.00	C
ATOM	2203	O	SER	C	53	37.336	11.388	36.166	1.00	26.97	O
ATOM	2204	CB	SER	C	53	38.172	8.499	37.198	1.00	25.64	C
ATOM	2205	OG	SER	C	53	38.902	8.772	36.019	1.00	24.45	O
ATOM	2206	N	ASP	C	54	35.544	10.421	36.932	1.00	27.50	N
ATOM	2207	CA	ASP	C	54	34.743	11.292	36.113	1.00	29.13	C
ATOM	2208	C	ASP	C	54	34.719	12.679	36.663	1.00	27.20	C
ATOM	2209	O	ASP	C	54	34.826	13.616	35.906	1.00	30.75	O
ATOM	2210	CB	ASP	C	54	33.314	10.874	36.099	1.00	35.74	C
ATOM	2211	CG	ASP	C	54	33.056	9.521	35.502	1.00	43.27	C
ATOM	2212	OD1	ASP	C	54	33.871	9.016	34.694	1.00	44.80	O
ATOM	2213	OD2	ASP	C	54	31.996	8.988	35.876	1.00	47.24	O
ATOM	2214	N	SER	C	55	34.554	12.829	37.966	1.00	26.41	N
ATOM	2215	CA	SER	C	55	34.470	14.119	38.610	1.00	23.34	C
ATOM	2216	C	SER	C	55	35.676	14.964	38.382	1.00	19.99	C
ATOM	2217	O	SER	C	55	35.544	16.157	38.175	1.00	20.42	O
ATOM	2218	CB	SER	C	55	34.306	13.948	40.105	1.00	24.40	C
ATOM	2219	OG	SER	C	55	33.079	13.321	40.431	1.00	24.29	O
ATOM	2220	N	LEU	C	56	36.837	14.339	38.432	1.00	19.40	N
ATOM	2221	CA	LEU	C	56	38.082	15.062	38.245	1.00	21.98	C
ATOM	2222	C	LEU	C	56	38.333	15.488	36.797	1.00	23.22	C
ATOM	2223	O	LEU	C	56	38.922	16.543	36.512	1.00	21.76	O
ATOM	2224	CB	LEU	C	56	39.301	14.271	38.793	1.00	21.06	C
ATOM	2225	CG	LEU	C	56	39.614	14.342	40.291	1.00	19.56	C
ATOM	2226	CD1	LEU	C	56	40.647	13.313	40.678	1.00	18.16	C

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FIGURE 8A-48

ATOM	2227	CD2	LEU	C	56	40.132	15.717	40.651	1.00	16.61	C
ATOM	2228	N	THR	C	57	37.873	14.624	35.881	1.00	25.77	N
ATOM	2229	CA	THR	C	57	37.991	14.906	34.462	1.00	28.23	C
ATOM	2230	C	THR	C	57	37.020	16.004	34.104	1.00	28.03	C
ATOM	2231	O	THR	C	57	37.390	16.908	33.364	1.00	31.55	O
ATOM	2232	CB	THR	C	57	37.813	13.669	33.596	1.00	30.08	C
ATOM	2233	OG1	THR	C	57	38.904	12.849	33.972	1.00	32.28	O
ATOM	2234	CG2	THR	C	57	38.044	13.945	32.109	1.00	33.98	C
ATOM	2235	N	ASP	C	58	35.831	16.009	34.675	1.00	26.77	N
ATOM	2236	CA	ASP	C	58	34.940	17.120	34.486	1.00	29.31	C
ATOM	2237	C	ASP	C	58	35.387	18.422	35.173	1.00	28.49	C
ATOM	2238	O	ASP	C	58	35.241	19.515	34.614	1.00	29.44	O
ATOM	2239	CB	ASP	C	58	33.489	16.679	34.870	1.00	36.00	C
ATOM	2240	CG	ASP	C	58	32.849	15.532	34.032	1.00	40.53	C
ATOM	2241	OD1	ASP	C	58	33.503	14.924	33.151	1.00	41.90	O
ATOM	2242	OD2	ASP	C	58	31.673	15.229	34.294	1.00	42.29	O
ATOM	2243	N	LEU	C	59	35.964	18.350	36.383	1.00	26.07	N
ATOM	2244	CA	LEU	C	59	36.486	19.508	37.074	1.00	21.52	C
ATOM	2245	C	LEU	C	59	37.611	20.115	36.285	1.00	19.04	C
ATOM	2246	O	LEU	C	59	37.748	21.317	36.312	1.00	20.31	O
ATOM	2247	CB	LEU	C	59	37.028	19.118	38.444	1.00	19.27	C
ATOM	2248	CG	LEU	C	59	37.519	20.223	39.377	1.00	18.52	C
ATOM	2249	CD1	LEU	C	59	36.411	21.181	39.805	1.00	14.85	C
ATOM	2250	CD2	LEU	C	59	38.147	19.538	40.574	1.00	18.90	C
ATOM	2251	N	LEU	C	60	38.399	19.348	35.553	1.00	19.17	N
ATOM	2252	CA	LEU	C	60	39.549	19.854	34.840	1.00	20.10	C
ATOM	2253	C	LEU	C	60	39.173	20.833	33.766	1.00	22.23	C
ATOM	2254	O	LEU	C	60	39.912	21.768	33.474	1.00	24.00	O
ATOM	2255	CB	LEU	C	60	40.290	18.718	34.206	1.00	18.56	C
ATOM	2256	CG	LEU	C	60	41.582	19.115	33.520	1.00	19.76	C
ATOM	2257	CD1	LEU	C	60	42.638	19.404	34.561	1.00	17.43	C
ATOM	2258	CD2	LEU	C	60	42.018	18.002	32.555	1.00	20.53	C
ATOM	2259	N	ASP	C	61	37.984	20.629	33.214	1.00	25.53	N
ATOM	2260	CA	ASP	C	61	37.471	21.478	32.157	1.00	27.32	C
ATOM	2261	C	ASP	C	61	36.950	22.809	32.666	1.00	24.92	C
ATOM	2262	O	ASP	C	61	36.768	23.738	31.883	1.00	26.04	O
ATOM	2263	CB	ASP	C	61	36.365	20.729	31.389	1.00	35.92	C
ATOM	2264	CG	ASP	C	61	36.753	19.367	30.759	1.00	45.09	C
ATOM	2265	OD1	ASP	C	61	37.808	19.241	30.086	1.00	48.21	O
ATOM	2266	OD2	ASP	C	61	35.970	18.414	30.956	1.00	49.47	O
ATOM	2267	N	LYS	C	62	36.733	22.956	33.979	1.00	22.12	N
ATOM	2268	CA	LYS	C	62	36.379	24.234	34.559	1.00	18.62	C
ATOM	2269	C	LYS	C	62	37.603	25.082	34.727	1.00	17.52	C
ATOM	2270	O	LYS	C	62	37.491	26.205	35.176	1.00	19.68	O
ATOM	2271	CB	LYS	C	62	35.718	24.064	35.888	1.00	17.21	C
ATOM	2272	CG	LYS	C	62	34.590	23.048	35.893	1.00	20.59	C
ATOM	2273	CD	LYS	C	62	33.552	23.302	34.802	1.00	23.94	C
ATOM	2274	CE	LYS	C	62	32.302	22.398	34.907	1.00	27.69	C
ATOM	2275	NZ	LYS	C	62	32.621	20.990	35.112	1.00	33.53	N
ATOM	2276	N	PHE	C	63	38.792	24.629	34.385	1.00	16.95	N
ATOM	2277	CA	PHE	C	63	39.980	25.398	34.650	1.00	18.75	C
ATOM	2278	C	PHE	C	63	40.714	25.584	33.363	1.00	20.52	C
ATOM	2279	O	PHE	C	63	40.491	24.894	32.375	1.00	22.83	O
ATOM	2280	CB	PHE	C	63	40.890	24.728	35.712	1.00	16.49	C
ATOM	2281	CG	PHE	C	63	40.280	24.790	37.109	1.00	15.86	C
ATOM	2282	CD1	PHE	C	63	40.413	25.931	37.893	1.00	15.21	C
ATOM	2283	CD2	PHE	C	63	39.475	23.764	37.555	1.00	16.14	C
ATOM	2284	CE1	PHE	C	63	39.717	26.070	39.078	1.00	11.64	C
ATOM	2285	CE2	PHE	C	63	38.742	23.932	38.732	1.00	17.01	C
ATOM	2286	CZ	PHE	C	63	38.864	25.086	39.487	1.00	11.68	C

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FIGURE 8A-49

ATOM	2287	N	SER	C	64	41.606	26.540	33.393	1.00	22.26
ATOM	2288	CA	SER	C	64	42.458	26.748	32.268	1.00	25.03
ATOM	2289	C	SER	C	64	43.928	26.724	32.651	1.00	27.32
ATOM	2290	O	SER	C	64	44.339	27.274	33.668	1.00	29.54
ATOM	2291	CB	SER	C	64	41.951	28.036	31.682	1.00	27.42
ATOM	2292	OG	SER	C	64	42.936	28.782	30.987	1.00	33.90
ATOM	2293	N	ASN	C	65	44.750	26.056	31.838	1.00	29.09
ATOM	2294	CA	ASN	C	65	46.183	25.967	32.048	1.00	29.94
ATOM	2295	C	ASN	C	65	46.912	27.280	31.894	1.00	31.16
ATOM	2296	O	ASN	C	65	46.482	28.228	31.252	1.00	32.15
ATOM	2297	CB	ASN	C	65	46.770	24.950	31.088	1.00	31.52
ATOM	2298	CG	ASN	C	65	48.076	24.325	31.558	1.00	31.71
ATOM	2299	OD1	ASN	C	65	48.626	24.591	32.636	1.00	30.12
ATOM	2300	ND2	ASN	C	65	48.554	23.457	30.676	1.00	32.43
ATOM	2301	N	ILE	C	66	48.053	27.328	32.558	1.00	34.70
ATOM	2302	CA	ILE	C	66	48.822	28.549	32.743	1.00	38.02
ATOM	2303	C	ILE	C	66	50.279	28.139	32.567	1.00	39.89
ATOM	2304	O	ILE	C	66	50.733	27.095	33.077	1.00	40.56
ATOM	2305	CB	ILE	C	66	48.560	29.130	34.181	1.00	37.96
ATOM	2306	CG1	ILE	C	66	47.097	29.513	34.381	1.00	37.79
ATOM	2307	CG2	ILE	C	66	49.443	30.334	34.443	1.00	37.53
ATOM	2308	CD1	ILE	C	66	46.677	29.759	35.833	1.00	39.98
ATOM	2309	N	SER	C	67	50.960	29.038	31.828	1.00	41.75
ATOM	2310	CA	SER	C	67	52.349	28.856	31.397	1.00	44.33
ATOM	2311	C	SER	C	67	53.320	28.647	32.536	1.00	44.00
ATOM	2312	O	SER	C	67	54.160	27.762	32.527	1.00	44.13
ATOM	2313	CB	SER	C	67	52.833	30.063	30.588	1.00	45.04
ATOM	2314	OG	SER	C	67	52.984	31.250	31.372	1.00	50.12
ATOM	2315	N	GLU	C	68	53.150	29.510	33.517	1.00	46.29
ATOM	2316	CA	GLU	C	68	53.969	29.520	34.702	1.00	49.75
ATOM	2317	C	GLU	C	68	53.215	29.731	36.043	1.00	48.90
ATOM	2318	O	GLU	C	68	52.374	30.624	36.267	1.00	49.09
ATOM	2319	CB	GLU	C	68	55.066	30.581	34.479	1.00	53.81
ATOM	2320	CG	GLU	C	68	56.220	30.174	33.547	1.00	59.46
ATOM	2321	CD	GLU	C	68	57.364	29.378	34.192	1.00	63.46
ATOM	2322	OE1	GLU	C	68	57.165	28.736	35.239	1.00	65.40
ATOM	2323	OE2	GLU	C	68	58.477	29.413	33.642	1.00	65.78
ATOM	2324	N	GLY	C	69	53.643	28.896	36.995	1.00	46.18
ATOM	2325	CA	GLY	C	69	52.938	28.734	38.244	1.00	41.09
ATOM	2326	C	GLY	C	69	52.252	27.398	38.142	1.00	37.69
ATOM	2327	O	GLY	C	69	51.845	26.975	37.057	1.00	38.22
ATOM	2328	N	LEU	C	70	52.181	26.712	39.279	1.00	34.58
ATOM	2329	CA	LEU	C	70	51.394	25.484	39.399	1.00	30.54
ATOM	2330	C	LEU	C	70	49.895	25.821	39.513	1.00	28.30
ATOM	2331	O	LEU	C	70	49.411	26.367	40.513	1.00	29.19
ATOM	2332	CB	LEU	C	70	51.895	24.714	40.615	1.00	28.69
ATOM	2333	CG	LEU	C	70	51.380	23.328	40.950	1.00	27.08
ATOM	2334	CD1	LEU	C	70	51.749	22.340	39.816	1.00	26.63
ATOM	2335	CD2	LEU	C	70	51.914	22.939	42.329	1.00	22.67
ATOM	2336	N	SER	C	71	49.173	25.536	38.430	1.00	23.37
ATOM	2337	CA	SER	C	71	47.795	25.909	38.342	1.00	18.79
ATOM	2338	C	SER	C	71	46.961	24.732	38.737	1.00	14.59
ATOM	2339	O	SER	C	71	47.420	23.616	38.830	1.00	13.92
ATOM	2340	CB	SER	C	71	47.499	26.362	36.929	1.00	19.04
ATOM	2341	OG	SER	C	71	47.794	25.282	36.073	1.00	21.34
ATOM	2342	N	ASN	C	72	45.691	25.004	38.938	1.00	15.21
ATOM	2343	CA	ASN	C	72	44.712	24.002	39.262	1.00	16.38
ATOM	2344	C	ASN	C	72	44.530	23.023	38.120	1.00	17.89
ATOM	2345	O	ASN	C	72	44.330	21.836	38.358	1.00	19.68
ATOM	2346	CB	ASN	C	72	43.395	24.668	39.627	1.00	14.20

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FIGURE 8A-50

ATOM	2347	CG	ASN	C	72	43.443	25.398	40.958	1.00 16.98
ATOM	2348	OD1	ASN	C	72	44.439	25.399	41.698	1.00 15.50
ATOM	2349	ND2	ASN	C	72	42.348	26.051	41.315	1.00 16.58
ATOM	2350	N	TYR	C	73	44.626	23.493	36.878	1.00 17.45
ATOM	2351	CA	TYR	C	73	44.546	22.649	35.715	1.00 16.35
ATOM	2352	C	TYR	C	73	45.628	21.603	35.846	1.00 16.88
ATOM	2353	O	TYR	C	73	45.388	20.407	35.803	1.00 18.90
ATOM	2354	CB	TYR	C	73	44.797	23.540	34.503	1.00 14.79
ATOM	2355	CG	TYR	C	73	44.618	22.779	33.215	1.00 18.01
ATOM	2356	CD1	TYR	C	73	45.649	22.000	32.745	1.00 18.75
ATOM	2357	CD2	TYR	C	73	43.428	22.809	32.544	1.00 17.80
ATOM	2358	CE1	TYR	C	73	45.507	21.189	31.632	1.00 23.12
ATOM	2359	CE2	TYR	C	73	43.282	22.000	31.424	1.00 23.77
ATOM	2360	CZ	TYR	C	73	44.300	21.160	30.987	1.00 22.85
ATOM	2361	OH	TYR	C	73	44.105	20.242	29.959	1.00 27.47
ATOM	2362	N	SER	C	74	46.846	22.071	36.054	1.00 19.27
ATOM	2363	CA	SER	C	74	48.037	21.234	36.196	1.00 18.80
ATOM	2364	C	SER	C	74	47.939	20.205	37.316	1.00 18.49
ATOM	2365	O	SER	C	74	48.192	19.026	37.062	1.00 18.14
ATOM	2366	CB	SER	C	74	49.160	22.197	36.410	1.00 19.97
ATOM	2367	OG	SER	C	74	50.345	21.552	36.749	1.00 27.05
ATOM	2368	N	ILE	C	75	47.536	20.603	38.532	1.00 17.15
ATOM	2369	CA	ILE	C	75	47.360	19.670	39.640	1.00 15.78
ATOM	2370	C	ILE	C	75	46.266	18.688	39.303	1.00 15.56
ATOM	2371	O	ILE	C	75	46.392	17.487	39.540	1.00 15.90
ATOM	2372	CB	ILE	C	75	47.004	20.373	40.994	1.00 14.47
ATOM	2373	CG1	ILE	C	75	48.069	21.396	41.311	1.00 15.08
ATOM	2374	CG2	ILE	C	75	46.847	19.406	42.151	1.00 9.44
ATOM	2375	CD1	ILE	C	75	47.662	22.494	42.334	1.00 16.06
ATOM	2376	N	ILE	C	76	45.174	19.165	38.739	1.00 15.87
ATOM	2377	CA	ILE	C	76	44.072	18.254	38.540	1.00 16.45
ATOM	2378	C	ILE	C	76	44.423	17.278	37.416	1.00 18.42
ATOM	2379	O	ILE	C	76	44.047	16.107	37.479	1.00 21.96
ATOM	2380	CB	ILE	C	76	42.777	19.029	38.276	1.00 16.99
ATOM	2381	CG1	ILE	C	76	42.407	20.014	39.366	1.00 18.36
ATOM	2382	CG2	ILE	C	76	41.661	18.026	38.294	1.00 18.72
ATOM	2383	CD1	ILE	C	76	41.376	21.090	38.981	1.00 13.71
ATOM	2384	N	ASP	C	77	45.169	17.686	36.395	1.00 19.28
ATOM	2385	CA	ASP	C	77	45.673	16.806	35.340	1.00 20.35
ATOM	2386	C	ASP	C	77	46.477	15.616	35.867	1.00 18.75
ATOM	2387	O	ASP	C	77	46.259	14.474	35.483	1.00 20.55
ATOM	2388	CB	ASP	C	77	46.528	17.679	34.388	1.00 23.72
ATOM	2389	CG	ASP	C	77	46.796	17.143	32.984	1.00 27.17
ATOM	2390	OD1	ASP	C	77	46.195	16.148	32.611	1.00 29.11
ATOM	2391	OD2	ASP	C	77	47.586	17.723	32.239	1.00 31.91
ATOM	2392	N	LYS	C	78	47.401	15.826	36.791	1.00 18.00
ATOM	2393	CA	LYS	C	78	48.064	14.729	37.494	1.00 19.18
ATOM	2394	C	LYS	C	78	47.114	13.802	38.229	1.00 16.84
ATOM	2395	O	LYS	C	78	47.200	12.586	38.170	1.00 18.34
ATOM	2396	CB	LYS	C	78	49.017	15.288	38.533	1.00 21.80
ATOM	2397	CG	LYS	C	78	50.492	15.453	38.249	1.00 26.26
ATOM	2398	CD	LYS	C	78	50.799	16.212	36.977	1.00 33.33
ATOM	2399	CE	LYS	C	78	51.977	17.190	37.154	1.00 36.36
ATOM	2400	NZ	LYS	C	78	51.538	18.516	37.592	1.00 40.57
ATOM	2401	N	LEU	C	79	46.160	14.358	38.937	1.00 17.71
ATOM	2402	CA	LEU	C	79	45.282	13.528	39.739	1.00 19.39
ATOM	2403	C	LEU	C	79	44.465	12.641	38.836	1.00 19.34
ATOM	2404	O	LEU	C	79	44.358	11.479	39.161	1.00 22.92
ATOM	2405	CB	LEU	C	79	44.412	14.342	40.708	1.00 15.20
ATOM	2406	CG	LEU	C	79	45.179	15.238	41.695	1.00 14.54

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FIGURE 8A-51

ATOM	2407	CD1	LEU	C	79	44.276	15.934	42.683	1.00	15.95
ATOM	2408	CD2	LEU	C	79	46.119	14.401	42.497	1.00	14.50
ATOM	2409	N	VAL	C	80	43.974	13.115	37.694	1.00	20.79
ATOM	2410	CA	VAL	C	80	43.210	12.349	36.719	1.00	19.75
ATOM	2411	C	VAL	C	80	44.068	11.231	36.229	1.00	20.92
ATOM	2412	O	VAL	C	80	43.583	10.133	36.160	1.00	19.45
ATOM	2413	CB	VAL	C	80	42.850	13.201	35.502	1.00	20.41
ATOM	2414	CG1	VAL	C	80	42.103	12.364	34.477	1.00	22.80
ATOM	2415	CG2	VAL	C	80	41.915	14.311	35.902	1.00	19.35
ATOM	2416	N	ASN	C	81	45.344	11.472	35.936	1.00	24.00
ATOM	2417	CA	ASN	C	81	46.215	10.435	35.447	1.00	24.32
ATOM	2418	C	ASN	C	81	46.460	9.366	36.474	1.00	25.83
ATOM	2419	O	ASN	C	81	46.405	8.188	36.168	1.00	27.41
ATOM	2420	CB	ASN	C	81	47.505	11.049	35.027	1.00	25.29
ATOM	2421	CG	ASN	C	81	47.389	11.689	33.658	1.00	27.98
ATOM	2422	OD1	ASN	C	81	47.347	10.977	32.667	1.00	30.37
ATOM	2423	ND2	ASN	C	81	47.387	13.000	33.477	1.00	27.47
ATOM	2424	N	ILE	C	82	46.690	9.750	37.714	1.00	27.31
ATOM	2425	CA	ILE	C	82	46.839	8.819	38.814	1.00	27.48
ATOM	2426	C	ILE	C	82	45.586	7.971	39.042	1.00	29.22
ATOM	2427	O	ILE	C	82	45.705	6.766	39.266	1.00	32.26
ATOM	2428	CB	ILE	C	82	47.228	9.685	40.022	1.00	26.77
ATOM	2429	CG1	ILE	C	82	48.662	10.131	39.852	1.00	24.85
ATOM	2430	CG2	ILE	C	82	47.046	8.977	41.344	1.00	26.49
ATOM	2431	CD1	ILE	C	82	49.159	11.193	40.833	1.00	24.34
ATOM	2432	N	VAL	C	83	44.371	8.547	38.968	1.00	30.80
ATOM	2433	CA	VAL	C	83	43.099	7.834	39.209	1.00	29.90
ATOM	2434	C	VAL	C	83	42.793	6.906	38.019	1.00	30.67
ATOM	2435	O	VAL	C	83	42.229	5.824	38.195	1.00	29.90
ATOM	2436	CB	VAL	C	83	41.888	8.816	39.455	1.00	27.23
ATOM	2437	CG1	VAL	C	83	40.651	8.141	39.973	1.00	28.89
ATOM	2438	CG2	VAL	C	83	42.154	9.759	40.558	1.00	28.33
ATOM	2439	N	ASP	C	84	43.174	7.298	36.797	1.00	31.05
ATOM	2440	CA	ASP	C	84	42.971	6.473	35.629	1.00	31.24
ATOM	2441	C	ASP	C	84	43.761	5.196	35.686	1.00	32.41
ATOM	2442	O	ASP	C	84	43.233	4.156	35.291	1.00	32.47
ATOM	2443	CB	ASP	C	84	43.296	7.192	34.350	1.00	31.90
ATOM	2444	CG	ASP	C	84	42.233	8.181	33.899	1.00	36.65
ATOM	2445	OD1	ASP	C	84	41.105	8.177	34.417	1.00	37.73
ATOM	2446	OD2	ASP	C	84	42.537	8.969	33.000	1.00	40.83
ATOM	2447	N	ASP	C	85	44.988	5.287	36.202	1.00	31.95
ATOM	2448	CA	ASP	C	85	45.770	4.128	36.589	1.00	34.69
ATOM	2449	C	ASP	C	85	45.189	3.114	37.564	1.00	34.70
ATOM	2450	O	ASP	C	85	45.464	1.921	37.471	1.00	34.86
ATOM	2451	CB	ASP	C	85	47.030	4.593	37.248	1.00	37.43
ATOM	2452	CG	ASP	C	85	48.101	5.028	36.290	1.00	41.26
ATOM	2453	OD1	ASP	C	85	47.860	4.978	35.077	1.00	45.93
ATOM	2454	OD2	ASP	C	85	49.169	5.423	36.776	1.00	43.39
ATOM	2455	N	LEU	C	86	44.445	3.587	38.552	1.00	34.35
ATOM	2456	CA	LEU	C	86	43.783	2.717	39.498	1.00	34.80
ATOM	2457	C	LEU	C	86	42.525	2.164	38.889	1.00	34.98
ATOM	2458	O	LEU	C	86	42.117	1.094	39.288	1.00	36.02
ATOM	2459	CB	LEU	C	86	43.443	3.508	40.735	1.00	35.24
ATOM	2460	CG	LEU	C	86	44.591	4.321	41.331	1.00	37.43
ATOM	2461	CD1	LEU	C	86	44.052	5.240	42.407	1.00	38.91
ATOM	2462	CD2	LEU	C	86	45.728	3.422	41.825	1.00	37.75
ATOM	2463	N	VAL	C	87	41.886	2.866	37.939	1.00	37.37
ATOM	2464	CA	VAL	C	87	40.748	2.365	37.175	1.00	38.56
ATOM	2465	C	VAL	C	87	41.236	1.205	36.320	1.00	41.43
ATOM	2466	O	VAL	C	87	40.621	0.154	36.337	1.00	43.44

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FIGURE 8A-52

ATOM	2467	CB	VAL	C	87	40.167	3.478	36.302	1.00	36.61	C
ATOM	2468	CG1	VAL	C	87	39.054	2.945	35.450	1.00	37.46	C
ATOM	2469	CG2	VAL	C	87	39.592	4.584	37.139	1.00	35.39	C
ATOM	2470	N	GLU	C	88	42.356	1.329	35.613	1.00	45.33	N
ATOM	2471	CA	GLU	C	88	42.933	0.237	34.842	1.00	50.04	C
ATOM	2472	C	GLU	C	88	43.480	-0.856	35.761	1.00	52.28	C
ATOM	2473	O	GLU	C	88	43.503	-2.015	35.374	1.00	53.46	O
ATOM	2474	CB	GLU	C	88	44.048	0.728	33.869	1.00	52.22	C
ATOM	2475	CG	GLU	C	88	43.776	1.785	32.749	1.00	56.99	C
ATOM	2476	CD	GLU	C	88	42.784	1.451	31.610	1.00	62.14	C
ATOM	2477	OE1	GLU	C	88	42.853	0.348	31.046	1.00	66.19	O
ATOM	2478	OE2	GLU	C	88	41.926	2.286	31.266	1.00	62.89	O
ATOM	2479	N	CYS	C	89	43.930	-0.535	36.982	1.00	55.77	N
ATOM	2480	CA	CYS	C	89	44.471	-1.508	37.936	1.00	58.72	C
ATOM	2481	C	CYS	C	89	43.372	-2.333	38.578	1.00	60.22	C
ATOM	2482	O	CYS	C	89	43.624	-3.464	39.000	1.00	61.13	O
ATOM	2483	CB	CYS	C	89	45.285	-0.819	39.048	1.00	59.69	C
ATOM	2484	SG	CYS	C	89	46.103	-1.924	40.239	1.00	65.48	S
ATOM	2485	N	VAL	C	90	42.159	-1.749	38.657	1.00	61.71	N
ATOM	2486	CA	VAL	C	90	40.963	-2.396	39.210	1.00	62.70	C
ATOM	2487	C	VAL	C	90	40.453	-3.516	38.278	1.00	64.64	C
ATOM	2488	O	VAL	C	90	40.010	-4.562	38.779	1.00	65.07	O
ATOM	2489	CB	VAL	C	90	39.934	-1.260	39.622	1.00	60.49	C
ATOM	2490	CG1	VAL	C	90	38.477	-1.428	39.231	1.00	58.30	C
ATOM	2491	CG2	VAL	C	90	40.023	-1.060	41.125	1.00	58.40	C
ATOM	2492	N	LYS	C	91	40.591	-3.348	36.938	1.00	66.41	N
ATOM	2493	CA	LYS	C	91	40.281	-4.402	35.971	1.00	68.79	C
ATOM	2494	C	LYS	C	91	41.219	-5.638	36.092	1.00	70.22	C
ATOM	2495	O	LYS	C	91	40.715	-6.728	36.404	1.00	72.46	O
ATOM	2496	CB	LYS	C	91	40.233	-3.836	34.530	1.00	68.55	C
ATOM	2497	CG	LYS	C	91	39.560	-4.821	33.535	1.00	71.09	C
ATOM	2498	CD	LYS	C	91	39.779	-4.534	32.028	1.00	71.78	C
ATOM	2499	CE	LYS	C	91	39.128	-3.245	31.514	1.00	70.74	C
ATOM	2500	NZ	LYS	C	91	39.730	-2.834	30.259	1.00	70.64	N
ATOM	2501	N	SER	C	104	25.399	2.470	38.962	1.00	56.13	N
ATOM	2502	CA	SER	C	104	25.444	3.921	38.739	1.00	55.65	C
ATOM	2503	C	SER	C	104	24.850	4.688	39.939	1.00	52.95	C
ATOM	2504	O	SER	C	104	23.647	4.968	39.947	1.00	53.89	O
ATOM	2505	CB	SER	C	104	24.797	4.326	37.337	1.00	57.16	C
ATOM	2506	OG	SER	C	104	23.517	3.792	36.940	1.00	56.67	O
ATOM	2507	N	PRO	C	105	25.618	5.024	41.000	1.00	49.29	N
ATOM	2508	CA	PRO	C	105	25.119	5.676	42.224	1.00	46.42	C
ATOM	2509	C	PRO	C	105	24.631	7.146	42.171	1.00	44.43	C
ATOM	2510	O	PRO	C	105	24.768	7.791	41.134	1.00	42.75	O
ATOM	2511	CB	PRO	C	105	26.265	5.445	43.181	1.00	45.66	C
ATOM	2512	CG	PRO	C	105	27.467	5.523	42.277	1.00	46.43	C
ATOM	2513	CD	PRO	C	105	27.036	4.706	41.089	1.00	47.56	C
ATOM	2514	N	GLU	C	106	24.023	7.707	43.240	1.00	44.38	N
ATOM	2515	CA	GLU	C	106	23.436	9.055	43.238	1.00	43.85	C
ATOM	2516	C	GLU	C	106	24.414	10.202	43.420	1.00	42.61	C
ATOM	2517	O	GLU	C	106	25.293	10.113	44.289	1.00	42.69	O
ATOM	2518	CB	GLU	C	106	22.321	9.281	44.289	1.00	45.50	C
ATOM	2519	CG	GLU	C	106	20.936	8.664	44.035	1.00	46.22	C
ATOM	2520	CD	GLU	C	106	20.404	8.761	42.607	1.00	45.82	C
ATOM	2521	OE1	GLU	C	106	20.257	9.861	42.067	1.00	41.34	O
ATOM	2522	OE2	GLU	C	106	20.152	7.699	42.032	1.00	48.83	O
ATOM	2523	N	PRO	C	107	24.254	11.291	42.632	1.00	41.36	N
ATOM	2524	CA	PRO	C	107	25.096	12.486	42.637	1.00	39.50	C
ATOM	2525	C	PRO	C	107	24.873	13.318	43.850	1.00	38.28	C
ATOM	2526	O	PRO	C	107	23.767	13.685	44.226	1.00	39.34	O

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FIGURE 8A-53

ATOM	2527	CB	PRO	C	107	24.680	13.288	41.434	1.00	40.28	C
ATOM	2528	CG	PRO	C	107	24.151	12.214	40.519	1.00	42.95	C
ATOM	2529	CD	PRO	C	107	23.353	11.358	41.490	1.00	41.93	N
ATOM	2530	N	ARG	C	108	26.012	13.570	44.436	1.00	35.97	C
ATOM	2531	CA	ARG	C	108	26.055	14.439	45.561	1.00	35.65	C
ATOM	2532	C	ARG	C	108	26.953	15.609	45.219	1.00	34.88	O
ATOM	2533	O	ARG	C	108	27.707	15.585	44.244	1.00	35.60	C
ATOM	2534	CB	ARG	C	108	26.617	13.701	46.756	1.00	39.40	C
ATOM	2535	CG	ARG	C	108	25.710	12.742	47.530	1.00	44.75	C
ATOM	2536	CD	ARG	C	108	25.959	12.906	49.053	1.00	48.86	N
ATOM	2537	NE	ARG	C	108	25.401	11.801	49.824	1.00	52.47	C
ATOM	2538	CZ	ARG	C	108	25.920	11.400	50.988	1.00	54.55	N
ATOM	2539	NH1	ARG	C	108	26.919	12.095	51.582	1.00	55.13	N
ATOM	2540	NH2	ARG	C	108	25.427	10.267	51.532	1.00	54.84	N
ATOM	2541	N	LEU	C	109	26.850	16.651	46.046	1.00	32.80	C
ATOM	2542	CA	LEU	C	109	27.686	17.851	45.949	1.00	31.31	C
ATOM	2543	C	LEU	C	109	28.544	17.984	47.198	1.00	27.53	O
ATOM	2544	O	LEU	C	109	28.058	17.849	48.335	1.00	29.28	C
ATOM	2545	CB	LEU	C	109	26.876	19.173	45.813	1.00	30.72	C
ATOM	2546	CG	LEU	C	109	25.837	19.411	44.752	1.00	29.60	C
ATOM	2547	CD1	LEU	C	109	25.143	20.697	45.150	1.00	31.86	C
ATOM	2548	CD2	LEU	C	109	26.433	19.432	43.347	1.00	30.24	N
ATOM	2549	N	PHE	C	110	29.841	18.247	46.995	1.00	24.61	C
ATOM	2550	CA	PHE	C	110	30.784	18.289	48.116	1.00	20.67	O
ATOM	2551	C	PHE	C	110	31.579	19.548	48.013	1.00	17.66	C
ATOM	2552	O	PHE	C	110	31.746	20.049	46.924	1.00	19.14	C
ATOM	2553	CB	PHE	C	110	31.721	17.098	48.021	1.00	23.08	C
ATOM	2554	CG	PHE	C	110	31.049	15.733	48.163	1.00	22.91	C
ATOM	2555	CD1	PHE	C	110	30.793	15.226	49.426	1.00	20.89	C
ATOM	2556	CD2	PHE	C	110	30.737	15.008	47.024	1.00	23.49	C
ATOM	2557	CE1	PHE	C	110	30.269	13.969	49.565	1.00	21.28	C
ATOM	2558	CE2	PHE	C	110	30.186	13.751	47.178	1.00	24.67	C
ATOM	2559	CZ	PHE	C	110	29.974	13.233	48.444	1.00	24.36	C
ATOM	2560	N	THR	C	111	32.071	20.116	49.084	1.00	17.78	N
ATOM	2561	CA	THR	C	111	32.961	21.249	48.978	1.00	18.25	C
ATOM	2562	C	THR	C	111	34.337	20.763	48.509	1.00	21.30	C
ATOM	2563	O	THR	C	111	34.518	19.547	48.617	1.00	26.22	O
ATOM	2564	CB	THR	C	111	33.057	21.895	50.359	1.00	19.78	C
ATOM	2565	OG1	THR	C	111	33.780	20.989	51.199	1.00	19.58	O
ATOM	2566	CG2	THR	C	111	31.663	22.215	50.913	1.00	18.93	O
ATOM	2567	N	PRO	C	112	35.360	21.512	48.024	1.00	19.29	N
ATOM	2568	CA	PRO	C	112	36.675	20.962	47.729	1.00	18.39	C
ATOM	2569	C	PRO	C	112	37.225	20.086	48.855	1.00	21.30	C
ATOM	2570	O	PRO	C	112	37.605	18.953	48.611	1.00	22.05	O
ATOM	2571	CB	PRO	C	112	37.455	22.226	47.520	1.00	18.00	C
ATOM	2572	CG	PRO	C	112	36.455	23.100	46.801	1.00	16.59	C
ATOM	2573	CD	PRO	C	112	35.265	22.919	47.660	1.00	14.34	N
ATOM	2574	N	GLU	C	113	37.221	20.521	50.119	1.00	22.83	C
ATOM	2575	CA	GLU	C	113	37.717	19.735	51.235	1.00	24.32	C
ATOM	2576	C	GLU	C	113	37.046	18.394	51.408	1.00	23.52	O
ATOM	2577	O	GLU	C	113	37.729	17.385	51.549	1.00	23.92	C
ATOM	2578	CB	GLU	C	113	37.496	20.463	52.524	1.00	27.24	C
ATOM	2579	CG	GLU	C	113	38.700	20.955	53.281	1.00	35.37	C
ATOM	2580	CD	GLU	C	113	38.282	21.200	54.724	1.00	39.80	O
ATOM	2581	OE1	GLU	C	113	37.915	20.230	55.387	1.00	41.11	O
ATOM	2582	OE2	GLU	C	113	38.296	22.339	55.182	1.00	41.53	N
ATOM	2583	N	GLU	C	114	35.712	18.350	51.386	1.00	23.35	C
ATOM	2584	CA	GLU	C	114	34.968	17.107	51.535	1.00	23.29	C
ATOM	2585	C	GLU	C	114	35.168	16.200	50.344	1.00	22.72	O
ATOM	2586	O	GLU	C	114	35.160	14.981	50.518	1.00	23.79	

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FIGURE 8A-54

ATOM	2587	CB	GLU	C	114	33.470	17.344	51.622	1.00	26.84	C
ATOM	2588	CG	GLU	C	114	32.974	18.114	52.849	1.00	31.67	C
ATOM	2589	CD	GLU	C	114	31.578	18.736	52.701	1.00	37.47	C
ATOM	2590	OE1	GLU	C	114	30.884	18.533	51.681	1.00	35.31	O
ATOM	2591	OE2	GLU	C	114	31.202	19.468	53.633	1.00	40.13	O
ATOM	2592	N	PHE	C	115	35.320	16.775	49.143	1.00	20.03	N
ATOM	2593	CA	PHE	C	115	35.606	15.979	47.971	1.00	18.15	C
ATOM	2594	C	PHE	C	115	36.997	15.397	48.157	1.00	17.33	C
ATOM	2595	O	PHE	C	115	37.214	14.205	48.013	1.00	18.05	O
ATOM	2596	CB	PHE	C	115	35.524	16.833	46.705	1.00	15.90	C
ATOM	2597	CG	PHE	C	115	35.825	16.063	45.429	1.00	17.09	C
ATOM	2598	CD1	PHE	C	115	34.861	15.299	44.845	1.00	16.21	C
ATOM	2599	CD2	PHE	C	115	37.094	16.093	44.890	1.00	18.64	C
ATOM	2600	CE1	PHE	C	115	35.193	14.558	43.744	1.00	19.14	C
ATOM	2601	CE2	PHE	C	115	37.425	15.336	43.795	1.00	18.76	C
ATOM	2602	CZ	PHE	C	115	36.463	14.570	43.217	1.00	19.41	C
ATOM	2603	N	PHE	C	116	38.010	16.167	48.509	1.00	19.36	N
ATOM	2604	CA	PHE	C	116	39.361	15.618	48.454	1.00	17.90	C
ATOM	2605	C	PHE	C	116	39.621	14.678	49.623	1.00	18.24	C
ATOM	2606	O	PHE	C	116	40.505	13.855	49.549	1.00	19.98	O
ATOM	2607	CB	PHE	C	116	40.376	16.744	48.162	1.00	16.33	C
ATOM	2608	CG	PHE	C	116	40.442	17.170	46.679	1.00	15.27	C
ATOM	2609	CD1	PHE	C	116	41.052	16.328	45.753	1.00	14.80	C
ATOM	2610	CD2	PHE	C	116	39.806	18.324	46.240	1.00	12.85	C
ATOM	2611	CE1	PHE	C	116	40.967	16.602	44.409	1.00	12.34	C
ATOM	2612	CE2	PHE	C	116	39.715	18.569	44.885	1.00	14.12	C
ATOM	2613	CZ	PHE	C	116	40.289	17.711	43.980	1.00	10.60	C
ATOM	2614	N	ARG	C	117	38.755	14.664	50.641	1.00	20.78	N
ATOM	2615	CA	ARG	C	117	38.796	13.751	51.770	1.00	21.33	C
ATOM	2616	C	ARG	C	117	38.412	12.368	51.308	1.00	20.46	C
ATOM	2617	O	ARG	C	117	39.076	11.405	51.639	1.00	21.70	O
ATOM	2618	CB	ARG	C	117	37.823	14.244	52.840	1.00	21.70	C
ATOM	2619	CG	ARG	C	117	37.838	13.513	54.177	1.00	27.63	C
ATOM	2620	CD	ARG	C	117	36.826	14.115	55.165	1.00	29.36	C
ATOM	2621	NE	ARG	C	117	37.230	15.464	55.616	1.00	32.11	N
ATOM	2622	CZ	ARG	C	117	36.411	16.535	55.565	1.00	32.37	C
ATOM	2623	NH1	ARG	C	117	35.179	16.464	55.047	1.00	32.61	N
ATOM	2624	NH2	ARG	C	117	36.836	17.701	56.025	1.00	30.98	N
ATOM	2625	N	ILE	C	118	37.342	12.263	50.540	1.00	21.91	N
ATOM	2626	CA	ILE	C	118	36.897	11.031	49.882	1.00	22.55	C
ATOM	2627	C	ILE	C	118	37.944	10.504	48.890	1.00	23.60	C
ATOM	2628	O	ILE	C	118	38.254	9.316	48.853	1.00	24.72	O
ATOM	2629	CB	ILE	C	118	35.527	11.358	49.213	1.00	22.47	C
ATOM	2630	CG1	ILE	C	118	34.467	11.506	50.293	1.00	21.67	C
ATOM	2631	CG2	ILE	C	118	35.117	10.338	48.161	1.00	21.48	C
ATOM	2632	CD1	ILE	C	118	33.164	12.169	49.825	1.00	21.12	C
ATOM	2633	N	PHE	C	119	38.544	11.402	48.103	1.00	23.86	N
ATOM	2634	CA	PHE	C	119	39.633	11.098	47.186	1.00	22.73	C
ATOM	2635	C	PHE	C	119	40.816	10.488	47.916	1.00	24.24	C
ATOM	2636	O	PHE	C	119	41.233	9.416	47.511	1.00	24.28	O
ATOM	2637	CB	PHE	C	119	40.038	12.357	46.426	1.00	15.88	C
ATOM	2638	CG	PHE	C	119	41.297	12.224	45.624	1.00	15.30	C
ATOM	2639	CD1	PHE	C	119	41.231	11.724	44.354	1.00	15.03	C
ATOM	2640	CD2	PHE	C	119	42.495	12.639	46.172	1.00	12.85	C
ATOM	2641	CE1	PHE	C	119	42.412	11.623	43.653	1.00	15.97	C
ATOM	2642	CE2	PHE	C	119	43.675	12.526	45.473	1.00	15.16	C
ATOM	2643	CZ	PHE	C	119	43.630	12.003	44.206	1.00	16.33	C
ATOM	2644	N	ASN	C	120	41.396	11.145	48.936	1.00	26.61	N
ATOM	2645	CA	ASN	C	120	42.511	10.621	49.728	1.00	27.10	C
ATOM	2646	C	ASN	C	120	42.225	9.301	50.400	1.00	28.31	C

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FIGURE 8A-55

ATOM	2647	O	ASN	C	120	43.081	8.433	50.376	1.00 28.63
ATOM	2648	CB	ASN	C	120	42.959	11.590	50.783	1.00 24.50
ATOM	2649	CG	ASN	C	120	43.837	12.659	50.215	1.00 27.34
ATOM	2650	OD1	ASN	C	120	43.864	13.757	50.761	1.00 27.34
ATOM	2651	ND2	ASN	C	120	44.628	12.420	49.169	1.00 29.64
ATOM	2652	N	ARG	C	121	41.017	9.136	50.947	1.00 30.80
ATOM	2653	CA	ARG	C	121	40.549	7.862	51.441	1.00 35.49
ATOM	2654	C	ARG	C	121	40.514	6.767	50.357	1.00 36.43
ATOM	2655	O	ARG	C	121	40.859	5.616	50.628	1.00 38.58
ATOM	2656	CB	ARG	C	121	39.202	8.108	52.138	1.00 37.63
ATOM	2657	CG	ARG	C	121	38.534	6.865	52.651	1.00 42.24
ATOM	2658	CD	ARG	C	121	37.240	7.194	53.373	1.00 47.82
ATOM	2659	NE	ARG	C	121	36.399	6.001	53.529	1.00 51.79
ATOM	2660	CZ	ARG	C	121	36.788	4.912	54.233	1.00 55.38
ATOM	2661	NH1	ARG	C	121	38.016	4.799	54.783	1.00 57.12
ATOM	2662	NH2	ARG	C	121	35.928	3.904	54.446	1.00 55.34
ATOM	2663	N	SER	C	122	40.171	7.089	49.106	1.00 36.49
ATOM	2664	CA	SER	C	122	40.274	6.177	47.974	1.00 36.44
ATOM	2665	C	SER	C	122	41.660	5.723	47.529	1.00 37.85
ATOM	2666	O	SER	C	122	41.874	4.556	47.235	1.00 39.23
ATOM	2667	CB	SER	C	122	39.613	6.814	46.788	1.00 34.58
ATOM	2668	OG	SER	C	122	38.286	7.132	47.155	1.00 34.47
ATOM	2669	N	ILE	C	123	42.638	6.599	47.409	1.00 38.85
ATOM	2670	CA	ILE	C	123	43.949	6.180	46.985	1.00 43.11
ATOM	2671	C	ILE	C	123	44.589	5.456	48.157	1.00 46.18
ATOM	2672	O	ILE	C	123	45.449	4.614	47.937	1.00 47.69
ATOM	2673	CB	ILE	C	123	44.843	7.378	46.505	1.00 42.65
ATOM	2674	CG1	ILE	C	123	44.147	8.410	45.599	1.00 38.38
ATOM	2675	CG2	ILE	C	123	46.146	6.866	45.872	1.00 43.09
ATOM	2676	CD1	ILE	C	123	43.242	7.872	44.489	1.00 35.80
ATOM	2677	N	ASP	C	124	44.206	5.755	49.402	1.00 50.61
ATOM	2678	CA	ASP	C	124	44.805	5.095	50.564	1.00 54.85
ATOM	2679	C	ASP	C	124	44.197	3.730	50.882	1.00 54.20
ATOM	2680	O	ASP	C	124	44.774	2.898	51.586	1.00 54.57
ATOM	2681	CB	ASP	C	124	44.788	5.989	51.823	1.00 59.47
ATOM	2682	CG	ASP	C	124	45.794	7.151	51.915	1.00 63.36
ATOM	2683	OD1	ASP	C	124	45.935	7.919	50.949	1.00 63.45
ATOM	2684	OD2	ASP	C	124	46.414	7.295	52.988	1.00 66.94
ATOM	2685	N	ALA	C	125	43.039	3.460	50.281	1.00 54.57
ATOM	2686	CA	ALA	C	125	42.427	2.137	50.314	1.00 56.99
ATOM	2687	C	ALA	C	125	43.150	1.108	49.440	1.00 58.85
ATOM	2688	O	ALA	C	125	42.617	0.022	49.161	1.00 59.46
ATOM	2689	CB	ALA	C	125	40.982	2.263	49.824	1.00 56.08
ATOM	2690	N	PHE	C	126	44.343	1.552	48.975	1.00 60.81
ATOM	2691	CA	PHE	C	126	45.408	0.793	48.316	1.00 62.82
ATOM	2692	C	PHE	C	126	46.675	0.603	49.241	1.00 64.91
ATOM	2693	O	PHE	C	126	47.801	0.492	48.731	1.00 65.88
ATOM	2694	CB	PHE	C	126	45.715	1.476	46.898	1.00 60.15
ATOM	2695	CG	PHE	C	126	44.638	1.419	45.778	1.00 57.55
ATOM	2696	CD1	PHE	C	126	43.594	2.334	45.731	1.00 56.09
ATOM	2697	CD2	PHE	C	126	44.655	0.421	44.813	1.00 56.90
ATOM	2698	CE1	PHE	C	126	42.568	2.227	44.807	1.00 52.24
ATOM	2699	CE2	PHE	C	126	43.627	0.319	43.884	1.00 54.42
ATOM	2700	CZ	PHE	C	126	42.573	1.208	43.889	1.00 52.99
TER	2702		PHE	C	126				
ATOM	2703	N	ASN	D	11	47.774	44.287	38.626	1.00 52.77
ATOM	2704	CA	ASN	D	11	46.416	43.904	38.273	1.00 53.01
ATOM	2705	C	ASN	D	11	46.383	43.039	36.995	1.00 52.04
ATOM	2706	O	ASN	D	11	46.673	41.852	37.139	1.00 53.30
ATOM	2707	CB	ASN	D	11	45.488	45.136	38.154	1.00 52.37

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FIGURE 8A-56

ATOM	2708	N	VAL	D	12	46.135	43.551	35.763	1.00 49.81	N
ATOM	2709	CA	VAL	D	12	45.936	42.823	34.490	1.00 45.10	C
ATOM	2710	C	VAL	D	12	46.697	41.529	34.194	1.00 40.73	O
ATOM	2711	O	VAL	D	12	46.109	40.477	33.958	1.00 39.20	C
ATOM	2712	CB	VAL	D	12	46.118	43.863	33.336	1.00 46.99	C
ATOM	2713	CG1	VAL	D	12	46.377	43.229	31.966	1.00 47.11	C
ATOM	2714	CG2	VAL	D	12	44.888	44.784	33.225	1.00 46.26	N
ATOM	2715	N	LYS	D	13	48.014	41.610	34.165	1.00 37.97	C
ATOM	2716	CA	LYS	D	13	48.844	40.432	34.132	1.00 36.45	C
ATOM	2717	C	LYS	D	13	48.402	39.322	35.117	1.00 36.18	O
ATOM	2718	O	LYS	D	13	48.194	38.166	34.709	1.00 37.38	C
ATOM	2719	CB	LYS	D	13	50.258	40.905	34.451	1.00 35.89	N
ATOM	2720	N	ASP	D	14	48.190	39.643	36.410	1.00 33.96	C
ATOM	2721	CA	ASP	D	14	47.703	38.684	37.372	1.00 29.22	C
ATOM	2722	C	ASP	D	14	46.220	38.409	37.305	1.00 25.55	O
ATOM	2723	O	ASP	D	14	45.799	37.316	37.647	1.00 25.36	C
ATOM	2724	CB	ASP	D	14	48.158	39.126	38.726	1.00 33.71	C
ATOM	2725	CG	ASP	D	14	49.573	38.623	39.084	1.00 41.45	O
ATOM	2726	OD1	ASP	D	14	50.178	37.858	38.316	1.00 45.64	O
ATOM	2727	OD2	ASP	D	14	50.083	38.981	40.161	1.00 44.73	N
ATOM	2728	N	VAL	D	15	45.421	39.347	36.809	1.00 22.15	C
ATOM	2729	CA	VAL	D	15	44.000	39.173	36.672	1.00 19.73	C
ATOM	2730	C	VAL	D	15	43.683	38.044	35.731	1.00 21.56	O
ATOM	2731	O	VAL	D	15	42.825	37.217	36.016	1.00 23.37	C
ATOM	2732	CB	VAL	D	15	43.294	40.462	36.234	1.00 18.49	C
ATOM	2733	CG1	VAL	D	15	41.883	40.238	35.684	1.00 17.31	C
ATOM	2734	CG2	VAL	D	15	43.093	41.327	37.450	1.00 17.77	N
ATOM	2735	N	THR	D	16	44.387	37.974	34.623	1.00 22.81	C
ATOM	2736	CA	THR	D	16	44.166	36.943	33.605	1.00 24.47	O
ATOM	2737	C	THR	D	16	44.517	35.513	34.082	1.00 21.91	C
ATOM	2738	O	THR	D	16	43.904	34.526	33.676	1.00 20.78	C
ATOM	2739	CB	THR	D	16	44.991	37.520	32.381	1.00 26.36	O
ATOM	2740	OG1	THR	D	16	44.076	38.310	31.630	1.00 28.31	C
ATOM	2741	CG2	THR	D	16	45.721	36.529	31.530	1.00 28.93	N
ATOM	2742	N	LYS	D	17	45.470	35.415	35.016	1.00 20.72	C
ATOM	2743	CA	LYS	D	17	45.958	34.179	35.596	1.00 20.21	C
ATOM	2744	C	LYS	D	17	45.019	33.719	36.683	1.00 18.63	O
ATOM	2745	O	LYS	D	17	44.754	32.526	36.783	1.00 21.04	C
ATOM	2746	CB	LYS	D	17	47.277	34.522	36.207	1.00 24.75	C
ATOM	2747	CG	LYS	D	17	48.163	33.373	36.590	1.00 29.44	C
ATOM	2748	CD	LYS	D	17	49.365	33.928	37.347	1.00 32.96	C
ATOM	2749	CE	LYS	D	17	50.423	34.474	36.422	1.00 36.20	N
ATOM	2750	NZ	LYS	D	17	51.313	35.272	37.230	1.00 39.87	N
ATOM	2751	N	LEU	D	18	44.483	34.656	37.468	1.00 16.11	C
ATOM	2752	CA	LEU	D	18	43.391	34.389	38.362	1.00 13.77	O
ATOM	2753	C	LEU	D	18	42.158	33.926	37.636	1.00 14.10	C
ATOM	2754	O	LEU	D	18	41.662	32.898	38.072	1.00 17.61	C
ATOM	2755	CB	LEU	D	18	43.070	35.599	39.180	1.00 14.87	C
ATOM	2756	CG	LEU	D	18	42.103	35.485	40.362	1.00 15.58	C
ATOM	2757	CD1	LEU	D	18	42.567	34.568	41.470	1.00 11.31	C
ATOM	2758	CD2	LEU	D	18	41.872	36.849	40.952	1.00 15.28	N
ATOM	2759	N	VAL	D	19	41.617	34.544	36.561	1.00 15.42	C
ATOM	2760	CA	VAL	D	19	40.479	34.034	35.786	1.00 13.39	C
ATOM	2761	C	VAL	D	19	40.704	32.587	35.385	1.00 14.30	O
ATOM	2762	O	VAL	D	19	39.824	31.744	35.542	1.00 13.93	C
ATOM	2763	CB	VAL	D	19	40.251	34.838	34.489	1.00 14.39	C
ATOM	2764	CG1	VAL	D	19	39.059	34.330	33.694	1.00 11.41	C
ATOM	2765	CG2	VAL	D	19	39.913	36.255	34.797	1.00 12.80	N
ATOM	2766	N	ALA	D	20	41.911	32.288	34.876	1.00 14.50	C
ATOM	2767	CA	ALA	D	20	42.319	30.924	34.543	1.00 15.90	C

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FIGURE 8A-57

ATOM	2768	C	ALA	D	20	42.340	29.894	35.680	1.00	16.27	C
ATOM	2769	O	ALA	D	20	42.153	28.697	35.464	1.00	14.91	O
ATOM	2770	CB	ALA	D	20	43.719	30.983	33.946	1.00	16.48	C
ATOM	2771	N	ASN	D	21	42.543	30.396	36.914	1.00	16.20	N
ATOM	2772	CA	ASN	D	21	42.665	29.549	38.081	1.00	14.59	C
ATOM	2773	C	ASN	D	21	41.408	29.513	38.923	1.00	15.22	C
ATOM	2774	O	ASN	D	21	41.343	28.894	39.982	1.00	14.76	O
ATOM	2775	CB	ASN	D	21	43.863	30.085	38.853	1.00	15.31	C
ATOM	2776	CG	ASN	D	21	44.760	29.000	39.360	1.00	12.22	C
ATOM	2777	OD1	ASN	D	21	45.002	28.023	38.669	1.00	15.31	O
ATOM	2778	ND2	ASN	D	21	45.313	29.122	40.545	1.00	14.81	N
ATOM	2779	N	LEU	D	22	40.364	30.201	38.493	1.00	15.62	N
ATOM	2780	CA	LEU	D	22	39.069	30.126	39.157	1.00	15.32	C
ATOM	2781	C	LEU	D	22	38.172	29.241	38.319	1.00	15.81	C
ATOM	2782	O	LEU	D	22	38.337	29.289	37.109	1.00	18.22	O
ATOM	2783	CB	LEU	D	22	38.470	31.498	39.326	1.00	11.04	C
ATOM	2784	CG	LEU	D	22	39.203	32.454	40.210	1.00	10.12	C
ATOM	2785	CD1	LEU	D	22	38.580	33.801	40.004	1.00	11.85	C
ATOM	2786	CD2	LEU	D	22	39.108	32.071	41.671	1.00	10.74	C
ATOM	2787	N	PRO	D	23	37.246	28.422	38.825	1.00	16.11	N
ATOM	2788	CA	PRO	D	23	36.365	27.588	38.004	1.00	15.30	C
ATOM	2789	C	PRO	D	23	35.533	28.456	37.064	1.00	16.55	C
ATOM	2790	O	PRO	D	23	35.044	29.485	37.502	1.00	18.78	O
ATOM	2791	CB	PRO	D	23	35.474	26.944	39.027	1.00	14.03	C
ATOM	2792	CG	PRO	D	23	36.252	27.043	40.317	1.00	16.22	C
ATOM	2793	CD	PRO	D	23	36.854	28.409	40.228	1.00	15.04	C
ATOM	2794	N	LYS	D	24	35.319	28.105	35.785	1.00	19.22	N
ATOM	2795	CA	LYS	D	24	34.492	28.864	34.822	1.00	19.57	C
ATOM	2796	C	LYS	D	24	33.027	28.975	35.241	1.00	18.94	C
ATOM	2797	O	LYS	D	24	32.381	29.956	34.910	1.00	22.65	O
ATOM	2798	CB	LYS	D	24	34.575	28.214	33.425	1.00	20.25	C
ATOM	2799	CG	LYS	D	24	35.853	28.425	32.655	1.00	19.83	C
ATOM	2800	CD	LYS	D	24	36.049	27.261	31.683	1.00	20.33	C
ATOM	2801	CE	LYS	D	24	37.542	27.297	31.291	1.00	25.04	C
ATOM	2802	NZ	LYS	D	24	38.019	26.084	30.623	1.00	27.36	N
ATOM	2803	N	ASP	D	25	32.490	28.011	36.007	1.00	20.97	N
ATOM	2804	CA	ASP	D	25	31.146	27.984	36.585	1.00	20.24	C
ATOM	2805	C	ASP	D	25	31.084	28.420	38.037	1.00	20.26	C
ATOM	2806	O	ASP	D	25	30.092	28.177	38.714	1.00	24.64	O
ATOM	2807	CB	ASP	D	25	30.557	26.555	36.502	1.00	21.95	C
ATOM	2808	CG	ASP	D	25	31.274	25.501	37.333	1.00	26.54	C
ATOM	2809	OD1	ASP	D	25	32.429	25.721	37.693	1.00	28.24	O
ATOM	2810	OD2	ASP	D	25	30.697	24.445	37.616	1.00	29.75	O
ATOM	2811	N	TYR	D	26	32.109	29.038	38.591	1.00	19.65	N
ATOM	2812	CA	TYR	D	26	31.978	29.716	39.865	1.00	19.99	C
ATOM	2813	C	TYR	D	26	31.327	31.078	39.666	1.00	20.55	C
ATOM	2814	O	TYR	D	26	31.837	31.882	38.892	1.00	23.24	O
ATOM	2815	CB	TYR	D	26	33.388	29.886	40.446	1.00	18.93	C
ATOM	2816	CG	TYR	D	26	33.487	30.459	41.844	1.00	18.30	C
ATOM	2817	CD1	TYR	D	26	32.718	29.938	42.855	1.00	17.48	C
ATOM	2818	CD2	TYR	D	26	34.309	31.538	42.057	1.00	19.75	C
ATOM	2819	CE1	TYR	D	26	32.689	30.542	44.078	1.00	17.10	C
ATOM	2820	CE2	TYR	D	26	34.304	32.124	43.291	1.00	21.03	C
ATOM	2821	CZ	TYR	D	26	33.494	31.613	44.276	1.00	19.84	C
ATOM	2822	OH	TYR	D	26	33.553	32.163	45.538	1.00	26.79	O
HETATM	2823	N	MSE	D	27	30.240	31.351	40.390	1.00	20.11	N
HETATM	2824	CA	MSE	D	27	29.563	32.640	40.409	1.00	19.68	C
HETATM	2825	C	MSE	D	27	29.972	33.547	41.554	1.00	19.24	C
HETATM	2826	O	MSE	D	27	29.844	33.217	42.722	1.00	18.84	O
HETATM	2827	CB	MSE	D	27	28.030	32.478	40.470	1.00	25.00	C

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FIGURE 8A-58

HETATM	2828	CG	MSE	D	27	27.356	31.633	39.361	1.00	27.34	C
HETATM	2829	SE	MSE	D	27	28.005	31.953	37.549	1.00	33.76	SE
HETATM	2830	CE	MSE	D	27	27.146	33.538	37.334	1.00	29.16	C
ATOM	2831	N	ILE	D	28	30.503	34.700	41.191	1.00	18.26	N
ATOM	2832	CA	ILE	D	28	30.838	35.733	42.127	1.00	18.98	C
ATOM	2833	C	ILE	D	28	29.668	36.703	42.239	1.00	19.61	C
ATOM	2834	O	ILE	D	28	29.151	37.088	41.196	1.00	22.18	O
ATOM	2835	CB	ILE	D	28	32.136	36.421	41.662	1.00	15.61	C
ATOM	2836	CG1	ILE	D	28	33.234	35.398	41.469	1.00	12.73	C
ATOM	2837	CG2	ILE	D	28	32.593	37.471	42.693	1.00	15.00	C
ATOM	2838	CD1	ILE	D	28	34.487	35.969	40.818	1.00	10.07	C
ATOM	2839	N	THR	D	29	29.199	37.105	43.433	1.00	20.30	N
ATOM	2840	CA	THR	D	29	28.142	38.118	43.587	1.00	18.55	C
ATOM	2841	C	THR	D	29	28.720	39.514	43.593	1.00	18.51	C
ATOM	2842	O	THR	D	29	29.681	39.757	44.305	1.00	20.24	O
ATOM	2843	CB	THR	D	29	27.248	37.915	44.853	1.00	18.42	C
ATOM	2844	OG1	THR	D	29	26.791	36.570	44.817	1.00	20.41	O
ATOM	2845	CG2	THR	D	29	25.982	38.747	44.836	1.00	16.39	C
ATOM	2846	N	LEU	D	30	28.205	40.455	42.785	1.00	18.52	N
ATOM	2847	CA	LEU	D	30	28.610	41.845	42.783	1.00	17.78	C
ATOM	2848	C	LEU	D	30	27.305	42.598	42.724	1.00	19.35	C
ATOM	2849	O	LEU	D	30	26.420	42.245	41.946	1.00	19.98	O
ATOM	2850	CB	LEU	D	30	29.390	42.149	41.505	1.00	18.28	C
ATOM	2851	CG	LEU	D	30	29.905	43.557	41.154	1.00	15.52	C
ATOM	2852	CD1	LEU	D	30	30.720	44.170	42.241	1.00	15.62	C
ATOM	2853	CD2	LEU	D	30	30.732	43.522	39.879	1.00	17.11	C
ATOM	2854	N	LYS	D	31	27.150	43.613	43.560	1.00	20.05	N
ATOM	2855	CA	LYS	D	31	26.046	44.522	43.409	1.00	21.35	C
ATOM	2856	C	LYS	D	31	26.413	45.564	42.354	1.00	23.46	C
ATOM	2857	O	LYS	D	31	27.223	46.470	42.561	1.00	23.96	O
ATOM	2858	CB	LYS	D	31	25.702	45.148	44.722	1.00	21.22	C
ATOM	2859	CG	LYS	D	31	25.353	44.109	45.766	1.00	23.53	C
ATOM	2860	CD	LYS	D	31	24.738	44.814	46.976	1.00	28.13	C
ATOM	2861	CE	LYS	D	31	24.583	43.890	48.182	1.00	29.07	C
ATOM	2862	NZ	LYS	D	31	23.982	44.617	49.293	1.00	34.24	N
ATOM	2863	N	TYR	D	32	25.818	45.356	41.172	1.00	25.01	N
ATOM	2864	CA	TYR	D	32	26.219	46.004	39.925	1.00	25.06	C
ATOM	2865	C	TYR	D	32	25.377	47.248	39.752	1.00	26.53	O
ATOM	2866	O	TYR	D	32	24.167	47.293	40.046	1.00	27.71	C
ATOM	2867	CB	TYR	D	32	26.050	44.978	38.778	1.00	25.42	C
ATOM	2868	CG	TYR	D	32	26.196	45.465	37.336	1.00	24.15	C
ATOM	2869	CD1	TYR	D	32	27.433	45.460	36.728	1.00	22.29	C
ATOM	2870	CD2	TYR	D	32	25.071	45.915	36.672	1.00	23.90	C
ATOM	2871	CE1	TYR	D	32	27.558	45.961	35.459	1.00	24.06	C
ATOM	2872	CE2	TYR	D	32	25.183	46.427	35.409	1.00	25.00	C
ATOM	2873	CZ	TYR	D	32	26.427	46.458	34.822	1.00	26.48	C
ATOM	2874	OH	TYR	D	32	26.533	47.012	33.558	1.00	26.81	O
ATOM	2875	N	VAL	D	33	26.099	48.297	39.333	1.00	28.52	N
ATOM	2876	CA	VAL	D	33	25.505	49.613	39.093	1.00	27.57	C
ATOM	2877	C	VAL	D	33	24.973	49.634	37.670	1.00	27.14	C
ATOM	2878	O	VAL	D	33	25.769	49.693	36.750	1.00	28.15	O
ATOM	2879	CB	VAL	D	33	26.529	50.724	39.288	1.00	26.82	C
ATOM	2880	CG1	VAL	D	33	25.931	52.066	38.921	1.00	25.83	C
ATOM	2881	CG2	VAL	D	33	26.880	50.758	40.755	1.00	25.22	C
ATOM	2882	N	PRO	D	34	23.674	49.548	37.434	1.00	27.51	N
ATOM	2883	CA	PRO	D	34	23.085	49.608	36.105	1.00	28.26	C
ATOM	2884	C	PRO	D	34	23.491	50.909	35.413	1.00	31.20	O
ATOM	2885	O	PRO	D	34	23.649	51.980	36.012	1.00	32.62	C
ATOM	2886	CB	PRO	D	34	21.617	49.574	36.407	1.00	27.82	C
ATOM	2887	CG	PRO	D	34	21.523	48.866	37.750	1.00	29.77	C

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FIGURE 8A-59

ATOM	2888	CD	PRO	D	34	22.668	49.494	38.488	1.00	27.97	C
ATOM	2889	N	GLY	D	35	23.756	50.780	34.117	1.00	32.89	N
ATOM	2890	CA	GLY	D	35	24.265	51.891	33.338	1.00	34.68	C
ATOM	2891	C	GLY	D	35	25.749	52.065	33.438	1.00	34.91	C
ATOM	2892	O	GLY	D	35	26.271	53.066	32.991	1.00	38.32	O
HETATM	2893	N	MSE	D	36	26.456	51.105	33.995	1.00	36.03	N
HETATM	2894	CA	MSE	D	36	27.910	51.084	34.060	1.00	38.11	C
HETATM	2895	C	MSE	D	36	28.634	51.193	32.726	1.00	38.57	C
HETATM	2896	O	MSE	D	36	29.741	51.717	32.594	1.00	39.99	O
HETATM	2897	CB	MSE	D	36	28.255	49.744	34.622	1.00	41.60	C
HETATM	2898	CG	MSE	D	36	28.972	49.795	35.911	1.00	45.00	SE
HETATM	2899	SE	MSE	D	36	30.412	48.532	35.745	1.00	54.90	SE
HETATM	2900	CE	MSE	D	36	30.966	48.492	33.897	1.00	45.21	C
ATOM	2901	N	ASP	D	37	27.956	50.571	31.760	1.00	39.01	N
ATOM	2902	CA	ASP	D	37	28.357	50.446	30.370	1.00	37.84	C
ATOM	2903	C	ASP	D	37	28.125	51.687	29.525	1.00	37.29	C
ATOM	2904	O	ASP	D	37	29.067	52.169	28.896	1.00	40.17	O
ATOM	2905	CB	ASP	D	37	27.725	49.194	29.760	1.00	37.35	C
ATOM	2906	CG	ASP	D	37	26.258	48.854	30.083	1.00	40.62	C
ATOM	2907	OD1	ASP	D	37	25.560	49.672	30.709	1.00	39.43	O
ATOM	2908	OD2	ASP	D	37	25.813	47.752	29.705	1.00	41.13	O
ATOM	2909	N	VAL	D	38	26.930	52.266	29.525	1.00	36.85	N
ATOM	2910	CA	VAL	D	38	26.665	53.462	28.719	1.00	38.43	C
ATOM	2911	C	VAL	D	38	27.021	54.828	29.311	1.00	39.02	C
ATOM	2912	O	VAL	D	38	27.395	55.748	28.581	1.00	39.83	O
ATOM	2913	CB	VAL	D	38	25.212	53.466	28.171	1.00	36.76	C
ATOM	2914	CG1	VAL	D	38	25.086	52.227	27.356	1.00	36.24	C
ATOM	2915	CG2	VAL	D	38	24.081	53.482	29.175	1.00	36.31	C
ATOM	2916	N	LEU	D	39	26.886	54.965	30.641	1.00	39.92	N
ATOM	2917	CA	LEU	D	39	27.031	56.231	31.341	1.00	38.96	C
ATOM	2918	C	LEU	D	39	28.495	56.624	31.625	1.00	41.40	C
ATOM	2919	O	LEU	D	39	29.397	55.777	31.589	1.00	40.82	O
ATOM	2920	CB	LEU	D	39	26.208	56.247	32.637	1.00	35.81	C
ATOM	2921	CG	LEU	D	39	24.706	56.030	32.689	1.00	34.18	C
ATOM	2922	CD1	LEU	D	39	24.285	56.206	34.141	1.00	33.76	C
ATOM	2923	CD2	LEU	D	39	23.900	56.980	31.827	1.00	31.66	C
ATOM	2924	N	PRO	D	40	28.807	57.926	31.852	1.00	44.17	N
ATOM	2925	CA	PRO	D	40	30.141	58.383	32.244	1.00	44.44	C
ATOM	2926	C	PRO	D	40	30.420	58.032	33.699	1.00	42.47	C
ATOM	2927	O	PRO	D	40	29.550	58.003	34.562	1.00	42.05	O
ATOM	2928	CB	PRO	D	40	30.115	59.908	32.011	1.00	45.14	C
ATOM	2929	CG	PRO	D	40	28.674	60.256	32.263	1.00	45.10	C
ATOM	2930	CD	PRO	D	40	27.934	59.092	31.603	1.00	46.22	C
ATOM	2931	N	SER	D	41	31.694	57.749	33.906	1.00	42.00	N
ATOM	2932	CA	SER	D	41	32.266	57.360	35.166	1.00	39.50	C
ATOM	2933	C	SER	D	41	31.724	58.115	36.365	1.00	38.61	C
ATOM	2934	O	SER	D	41	31.345	57.439	37.303	1.00	38.99	O
ATOM	2935	CB	SER	D	41	33.760	57.491	35.009	1.00	40.43	C
ATOM	2936	OG	SER	D	41	34.204	56.814	33.824	1.00	45.16	O
ATOM	2937	N	HIS	D	42	31.550	59.442	36.396	1.00	38.17	N
ATOM	2938	CA	HIS	D	42	31.018	60.127	37.567	1.00	36.99	C
ATOM	2939	C	HIS	D	42	29.633	59.685	38.068	1.00	38.51	C
ATOM	2940	O	HIS	D	42	29.219	59.978	39.190	1.00	39.73	O
ATOM	2941	CB	HIS	D	42	31.062	61.646	37.328	1.00	36.53	C
ATOM	2942	CG	HIS	D	42	29.988	62.146	36.370	1.00	34.40	C
ATOM	2943	ND1	HIS	D	42	30.070	62.275	35.063	1.00	35.82	N
ATOM	2944	CD2	HIS	D	42	28.694	62.443	36.749	1.00	36.22	C
ATOM	2945	CE1	HIS	D	42	28.872	62.607	34.629	1.00	35.92	C
ATOM	2946	NE2	HIS	D	42	28.050	62.680	35.644	1.00	37.56	N
ATOM	2947	N	CYS	D	43	28.848	58.974	37.261	1.00	40.38	N

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FIGURE 8A-60

ATOM	2948	CA	CYS	D	43	27.521	58.516	37.662	1.00	40.95	C
ATOM	2949	C	CYS	D	43	27.545	57.165	38.394	1.00	38.66	C
ATOM	2950	O	CYS	D	43	26.556	56.769	39.027	1.00	38.58	O
ATOM	2951	CB	CYS	D	43	26.561	58.489	36.426	1.00	43.16	C
ATOM	2952	SG	CYS	D	43	25.889	60.126	35.971	1.00	50.07	S
ATOM	2953	N	TRP	D	44	28.677	56.450	38.300	1.00	34.96	N
ATOM	2954	CA	TRP	D	44	28.763	55.094	38.789	1.00	32.27	C
ATOM	2955	C	TRP	D	44	30.055	54.754	39.486	1.00	32.35	C
ATOM	2956	O	TRP	D	44	30.010	53.891	40.349	1.00	34.30	O
ATOM	2957	CB	TRP	D	44	28.502	54.045	37.688	1.00	29.74	C
ATOM	2958	CG	TRP	D	44	29.428	54.039	36.479	1.00	25.62	C
ATOM	2959	CD1	TRP	D	44	29.034	54.689	35.340	1.00	24.56	C
ATOM	2960	CD2	TRP	D	44	30.636	53.392	36.360	1.00	24.29	C
ATOM	2961	NE1	TRP	D	44	30.006	54.462	34.497	1.00	26.57	N
ATOM	2962	CE2	TRP	D	44	30.972	53.705	35.046	1.00	25.16	C
ATOM	2963	CE3	TRP	D	44	31.442	52.536	37.072	1.00	21.05	C
ATOM	2964	CZ2	TRP	D	44	32.119	53.210	34.446	1.00	23.57	C
ATOM	2965	CZ3	TRP	D	44	32.600	52.058	36.490	1.00	21.72	C
ATOM	2966	CH2	TRP	D	44	32.956	52.395	35.194	1.00	23.72	C
ATOM	2967	N	ILE	D	45	31.191	55.378	39.216	1.00	31.34	N
ATOM	2968	CA	ILE	D	45	32.444	54.851	39.687	1.00	34.23	C
ATOM	2969	C	ILE	D	45	32.627	54.719	41.206	1.00	35.04	C
ATOM	2970	O	ILE	D	45	33.222	53.726	41.618	1.00	36.05	O
ATOM	2971	CB	ILE	D	45	33.586	55.584	38.980	1.00	35.62	C
ATOM	2972	CG1	ILE	D	45	34.959	54.917	39.068	1.00	36.05	C
ATOM	2973	CG2	ILE	D	45	33.716	56.959	39.592	1.00	37.86	C
ATOM	2974	CD1	ILE	D	45	35.020	53.482	38.545	1.00	36.81	C
ATOM	2975	N	SER	D	46	32.100	55.591	42.080	1.00	35.07	N
ATOM	2976	CA	SER	D	46	32.421	55.538	43.500	1.00	35.85	C
ATOM	2977	C	SER	D	46	31.651	54.443	44.213	1.00	35.51	C
ATOM	2978	O	SER	D	46	32.169	53.858	45.165	1.00	38.41	O
ATOM	2979	CB	SER	D	46	32.165	56.852	44.223	1.00	36.96	C
ATOM	2980	OG	SER	D	46	30.786	57.005	44.534	1.00	40.12	O
ATOM	2981	N	GLU	D	47	30.419	54.185	43.770	1.00	33.93	N
ATOM	2982	CA	GLU	D	47	29.656	53.051	44.230	1.00	32.65	C
ATOM	2983	C	GLU	D	47	30.197	51.773	43.648	1.00	31.56	C
ATOM	2984	O	GLU	D	47	30.216	50.761	44.339	1.00	31.25	O
ATOM	2985	CB	GLU	D	47	28.206	53.193	43.842	1.00	36.42	C
ATOM	2986	CG	GLU	D	47	27.306	51.989	44.164	1.00	45.32	C
ATOM	2987	CD	GLU	D	47	26.964	51.716	45.628	1.00	48.90	C
ATOM	2988	OE1	GLU	D	47	27.839	51.323	46.399	1.00	52.24	O
ATOM	2989	OE2	GLU	D	47	25.797	51.872	45.995	1.00	52.95	O
HETATM	2990	N	MSE	D	48	30.646	51.788	42.398	1.00	30.45	N
HETATM	2991	CA	MSE	D	48	31.189	50.592	41.798	1.00	31.67	C
HETATM	2992	C	MSE	D	48	32.499	50.155	42.444	1.00	30.88	C
HETATM	2993	O	MSE	D	48	32.694	48.961	42.577	1.00	33.46	O
HETATM	2994	CB	MSE	D	48	31.394	50.777	40.342	1.00	32.74	C
HETATM	2995	CG	MSE	D	48	31.510	49.459	39.632	1.00	36.29	C
HETATM	2996	SE	MSE	D	48	29.910	48.366	39.787	1.00	47.34	SE
HETATM	2997	CE	MSE	D	48	30.895	46.927	39.264	1.00	38.75	C
ATOM	2998	N	VAL	D	49	33.433	50.984	42.904	1.00	30.60	N
ATOM	2999	CA	VAL	D	49	34.605	50.504	43.671	1.00	29.47	C
ATOM	3000	C	VAL	D	49	34.285	50.012	45.074	1.00	27.89	C
ATOM	3001	O	VAL	D	49	34.967	49.128	45.596	1.00	27.63	O
ATOM	3002	CB	VAL	D	49	35.828	51.488	43.781	1.00	30.38	C
ATOM	3003	CG1	VAL	D	49	36.552	51.617	42.439	1.00	30.57	C
ATOM	3004	CG2	VAL	D	49	35.440	52.863	44.340	1.00	30.43	C
ATOM	3005	N	VAL	D	50	33.263	50.622	45.679	1.00	25.21	N
ATOM	3006	CA	VAL	D	50	32.754	50.149	46.945	1.00	24.70	C
ATOM	3007	C	VAL	D	50	32.153	48.745	46.832	1.00	24.08	C

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FIGURE 8A-61

ATOM	3008	O	VAL	D	50	32.438	47.921	47.699	1.00	25.08		O
ATOM	3009	CB	VAL	D	50	31.757	51.172	47.504	1.00	24.15		C
ATOM	3010	CG1	VAL	D	50	30.945	50.583	48.650	1.00	24.85		C
ATOM	3011	CG2	VAL	D	50	32.484	52.411	47.974	1.00	21.01		C
ATOM	3012	N	GLN	D	51	31.343	48.470	45.796	1.00	22.06		N
ATOM	3013	CA	GLN	D	51	30.807	47.154	45.522	1.00	22.13		C
ATOM	3014	C	GLN	D	51	31.810	46.099	45.123	1.00	20.89		C
ATOM	3015	O	GLN	D	51	31.663	44.940	45.479	1.00	21.33		O
ATOM	3016	CB	GLN	D	51	29.719	47.249	44.484	1.00	24.57		C
ATOM	3017	CG	GLN	D	51	28.496	47.999	45.018	1.00	26.12		C
ATOM	3018	CD	GLN	D	51	27.936	47.379	46.304	1.00	26.75		C
ATOM	3019	OE1	GLN	D	51	28.128	46.194	46.616	1.00	25.54		O
ATOM	3020	NE2	GLN	D	51	27.234	48.198	47.088	1.00	26.23		N
ATOM	3021	N	LEU	D	52	32.839	46.544	44.423	1.00	19.69		N
ATOM	3022	CA	LEU	D	52	33.966	45.728	44.057	1.00	20.34		C
ATOM	3023	C	LEU	D	52	34.831	45.383	45.250	1.00	20.47		C
ATOM	3024	O	LEU	D	52	35.199	44.215	45.356	1.00	23.75		O
ATOM	3025	CB	LEU	D	52	34.866	46.398	42.976	1.00	19.72		C
ATOM	3026	CG	LEU	D	52	34.402	46.541	41.509	1.00	18.02		C
ATOM	3027	CD1	LEU	D	52	35.404	47.412	40.807	1.00	14.47		C
ATOM	3028	CD2	LEU	D	52	34.217	45.177	40.844	1.00	14.93		C
ATOM	3029	N	SER	D	53	35.178	46.294	46.165	1.00	21.36		N
ATOM	3030	CA	SER	D	53	35.913	45.942	47.377	1.00	22.45		C
ATOM	3031	C	SER	D	53	35.173	44.873	48.166	1.00	22.70		C
ATOM	3032	O	SER	D	53	35.770	43.895	48.565	1.00	24.55		O
ATOM	3033	CB	SER	D	53	36.117	47.178	48.233	1.00	25.43		C
ATOM	3034	OG	SER	D	53	36.882	46.917	49.410	1.00	32.17		O
ATOM	3035	N	ASP	D	54	33.852	44.962	48.286	1.00	23.74		N
ATOM	3036	CA	ASP	D	54	33.021	44.038	49.030	1.00	25.51		C
ATOM	3037	C	ASP	D	54	33.119	42.633	48.500	1.00	22.56		C
ATOM	3038	O	ASP	D	54	33.390	41.711	49.250	1.00	22.33		O
ATOM	3039	CB	ASP	D	54	31.565	44.500	48.963	1.00	32.00		C
ATOM	3040	CG	ASP	D	54	30.624	43.913	50.019	1.00	42.23		C
ATOM	3041	OD1	ASP	D	54	30.117	42.792	49.841	1.00	45.21		O
ATOM	3042	OD2	ASP	D	54	30.364	44.607	51.018	1.00	49.94		O
ATOM	3043	N	SER	D	55	32.943	42.520	47.192	1.00	19.99		N
ATOM	3044	CA	SER	D	55	32.933	41.258	46.504	1.00	16.42		C
ATOM	3045	C	SER	D	55	34.279	40.596	46.521	1.00	14.71		C
ATOM	3046	O	SER	D	55	34.395	39.393	46.693	1.00	15.83		O
ATOM	3047	CB	SER	D	55	32.503	41.468	45.066	1.00	16.29		C
ATOM	3048	OG	SER	D	55	31.170	41.909	44.886	1.00	19.97		O
ATOM	3049	N	LEU	D	56	35.296	41.406	46.315	1.00	15.85		N
ATOM	3050	CA	LEU	D	56	36.638	40.884	46.345	1.00	17.57		C
ATOM	3051	C	LEU	D	56	37.034	40.485	47.744	1.00	17.75		C
ATOM	3052	O	LEU	D	56	37.782	39.527	47.863	1.00	19.01		O
ATOM	3053	CB	LEU	D	56	37.619	41.904	45.848	1.00	17.61		C
ATOM	3054	CG	LEU	D	56	37.813	42.091	44.344	1.00	21.27		C
ATOM	3055	CD1	LEU	D	56	38.577	43.396	44.141	1.00	19.96		C
ATOM	3056	CD2	LEU	D	56	38.540	40.936	43.687	1.00	16.32		C
ATOM	3057	N	THR	D	57	36.560	41.169	48.803	1.00	19.07		N
ATOM	3058	CA	THR	D	57	36.864	40.818	50.189	1.00	17.97		C
ATOM	3059	C	THR	D	57	36.126	39.571	50.566	1.00	18.20		C
ATOM	3060	O	THR	D	57	36.674	38.746	51.266	1.00	20.89		O
ATOM	3061	CB	THR	D	57	36.521	41.984	51.099	1.00	19.37		C
ATOM	3062	OG1	THR	D	57	37.503	42.932	50.741	1.00	20.91		O
ATOM	3063	CG2	THR	D	57	36.778	41.786	52.575	1.00	26.13		C
ATOM	3064	N	ASP	D	58	34.924	39.346	50.085	1.00	18.03		N
ATOM	3065	CA	ASP	D	58	34.293	38.066	50.220	1.00	18.76		C
ATOM	3066	C	ASP	D	58	34.958	37.009	49.397	1.00	20.46		C
ATOM	3067	O	ASP	D	58	35.041	35.878	49.865	1.00	20.47		O

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FIGURE 8A-62

ATOM	3068	CB	ASP	D	58	32.859	38.102	49.791	1.00	21.24	
ATOM	3069	CG	ASP	D	58	32.043	39.157	50.517	1.00	26.19	C
ATOM	3070	OD1	ASP	D	58	32.458	39.665	51.572	1.00	26.83	O
ATOM	3071	OD2	ASP	D	58	30.970	39.481	49.993	1.00	30.50	N
ATOM	3072	N	LEU	D	59	35.449	37.324	48.197	1.00	19.65	C
ATOM	3073	CA	LEU	D	59	36.099	36.331	47.383	1.00	18.09	C
ATOM	3074	C	LEU	D	59	37.345	35.878	48.090	1.00	19.12	O
ATOM	3075	O	LEU	D	59	37.553	34.694	48.251	1.00	23.04	C
ATOM	3076	CB	LEU	D	59	36.392	36.893	46.028	1.00	16.75	C
ATOM	3077	CG	LEU	D	59	36.808	35.864	45.048	1.00	17.14	C
ATOM	3078	CD1	LEU	D	59	35.714	34.823	44.909	1.00	16.41	C
ATOM	3079	CD2	LEU	D	59	37.209	36.546	43.769	1.00	16.93	N
ATOM	3080	N	LEU	D	60	38.132	36.764	48.667	1.00	21.47	C
ATOM	3081	CA	LEU	D	60	39.332	36.428	49.431	1.00	22.73	C
ATOM	3082	C	LEU	D	60	39.173	35.401	50.564	1.00	24.38	O
ATOM	3083	O	LEU	D	60	40.084	34.626	50.853	1.00	25.12	C
ATOM	3084	CB	LEU	D	60	39.852	37.726	50.017	1.00	21.70	C
ATOM	3085	CG	LEU	D	60	41.196	37.710	50.670	1.00	23.77	C
ATOM	3086	CD1	LEU	D	60	42.256	37.514	49.598	1.00	22.63	C
ATOM	3087	CD2	LEU	D	60	41.446	38.985	51.425	1.00	24.99	C
ATOM	3088	N	ASP	D	61	38.005	35.386	51.224	1.00	26.63	N
ATOM	3089	CA	ASP	D	61	37.705	34.524	52.363	1.00	25.59	C
ATOM	3090	C	ASP	D	61	37.428	33.112	51.872	1.00	22.43	O
ATOM	3091	O.	ASP	D	61	37.373	32.161	52.646	1.00	23.39	C
ATOM	3092	CB	ASP	D	61	36.497	35.146	53.120	1.00	33.33	C
ATOM	3093	CG	ASP	D	61	35.889	34.390	54.325	1.00	40.36	C
ATOM	3094	OD1	ASP	D	61	36.478	34.403	55.424	1.00	44.78	O
ATOM	3095	OD2	ASP	D	61	34.807	33.794	54.169	1.00	43.10	N
ATOM	3096	N	LYS	D	62	37.289	32.899	50.575	1.00	17.94	C
ATOM	3097	CA	LYS	D	62	37.048	31.574	50.058	1.00	13.29	C
ATOM	3098	C	LYS	D	62	38.344	30.855	49.757	1.00	12.68	O
ATOM	3099	O	LYS	D	62	38.308	29.692	49.387	1.00	15.69	C
ATOM	3100	CB	LYS	D	62	36.292	31.712	48.771	1.00	13.99	C
ATOM	3101	CG	LYS	D	62	35.036	32.517	48.890	1.00	16.25	C
ATOM	3102	CD	LYS	D	62	34.086	31.871	49.870	1.00	21.21	C
ATOM	3103	CE	LYS	D	62	32.997	32.898	50.166	1.00	23.50	C
ATOM	3104	NZ	LYS	D	62	32.319	33.267	48.937	1.00	30.45	N
ATOM	3105	N	PHE	D	63	39.504	31.504	49.885	1.00	12.18	C
ATOM	3106	CA	PHE	D	63	40.797	30.938	49.594	1.00	13.29	O
ATOM	3107	C	PHE	D	63	41.659	30.965	50.837	1.00	16.38	C
ATOM	3108	O	PHE	D	63	41.401	31.701	51.798	1.00	16.40	C
ATOM	3109	CB	PHE	D	63	41.495	31.773	48.552	1.00	11.01	C
ATOM	3110	CG	PHE	D	63	40.776	31.641	47.229	1.00	13.33	C
ATOM	3111	CD1	PHE	D	63	40.917	30.478	46.491	1.00	11.26	C
ATOM	3112	CD2	PHE	D	63	39.904	32.635	46.823	1.00	13.18	C
ATOM	3113	CE1	PHE	D	63	40.140	30.299	45.367	1.00	9.84	C
ATOM	3114	CE2	PHE	D	63	39.126	32.436	45.690	1.00	13.90	C
ATOM	3115	CZ	PHE	D	63	39.251	31.264	44.964	1.00	10.53	N
ATOM	3116	N	SER	D	64	42.725	30.164	50.773	1.00	16.82	C
ATOM	3117	CA	SER	D	64	43.703	30.208	51.822	1.00	16.74	C
ATOM	3118	C	SER	D	64	45.123	30.230	51.275	1.00	16.89	O
ATOM	3119	O	SER	D	64	45.377	29.918	50.120	1.00	16.97	C
ATOM	3120	CB	SER	D	64	43.430	29.068	52.849	1.00	18.93	C
ATOM	3121	OG	SER	D	64	44.080	27.847	52.508	1.00	28.24	O
ATOM	3122	N	ASN	D	65	46.080	30.661	52.095	1.00	16.96	N
ATOM	3123	CA	ASN	D	65	47.479	30.684	51.746	1.00	15.98	C
ATOM	3124	C	ASN	D	65	48.027	29.319	51.496	1.00	15.15	C
ATOM	3125	O	ASN	D	65	47.472	28.362	52.000	1.00	17.07	O
ATOM	3126	CB	ASN	D	65	48.341	31.398	52.774	1.00	17.48	C
ATOM	3127	CG	ASN	D	65	48.232	32.904	52.684	1.00	19.71	C

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FIGURE 8A-63

ATOM	3128	OD1	ASN	D	65	48.695	33.551	51.752	1.00	25.73	O
ATOM	3129	ND2	ASN	D	65	47.621	33.560	53.640	1.00	22.21	N
ATOM	3130	N	ILE	D	66	49.077	29.253	50.672	1.00	15.61	N
ATOM	3131	CA	ILE	D	66	49.778	28.029	50.363	1.00	16.53	C
ATOM	3132	C	ILE	D	66	51.232	28.235	50.711	1.00	16.49	C
ATOM	3133	O	ILE	D	66	51.633	29.383	50.813	1.00	17.79	O
ATOM	3134	CB	ILE	D	66	49.594	27.623	48.869	1.00	16.19	C
ATOM	3135	CG1	ILE	D	66	50.149	28.660	47.906	1.00	16.66	C
ATOM	3136	CG2	ILE	D	66	48.115	27.329	48.611	1.00	12.63	C
ATOM	3137	CD1	ILE	D	66	50.081	28.086	46.478	1.00	18.10	N
ATOM	3138	N	SER	D	67	52.041	27.187	50.853	1.00	18.84	C
ATOM	3139	CA	SER	D	67	53.442	27.347	51.233	1.00	23.17	C
ATOM	3140	C	SER	D	67	54.305	28.078	50.214	1.00	23.34	O
ATOM	3141	O	SER	D	67	55.250	28.779	50.552	1.00	25.92	C
ATOM	3142	CB	SER	D	67	54.084	26.006	51.543	1.00	23.00	O
ATOM	3143	OG	SER	D	67	53.971	25.139	50.419	1.00	30.06	N
ATOM	3144	N	GLU	D	68	53.981	27.968	48.942	1.00	25.32	C
ATOM	3145	CA	GLU	D	68	54.755	28.626	47.914	1.00	27.08	C
ATOM	3146	C	GLU	D	68	54.045	28.401	46.597	1.00	25.08	O
ATOM	3147	O	GLU	D	68	53.391	27.373	46.403	1.00	24.26	C
ATOM	3148	CB	GLU	D	68	56.190	28.061	47.921	1.00	30.32	C
ATOM	3149	CG	GLU	D	68	56.711	27.081	46.883	1.00	40.98	O
ATOM	3150	CD	GLU	D	68	56.009	25.744	46.778	1.00	46.80	N
ATOM	3151	OE1	GLU	D	68	55.947	24.998	47.773	1.00	50.12	C
ATOM	3152	OE2	GLU	D	68	55.508	25.470	45.676	1.00	52.68	O
ATOM	3153	N	GLY	D	69	54.121	29.389	45.723	1.00	23.65	N
ATOM	3154	CA	GLY	D	69	53.784	29.192	44.320	1.00	24.95	C
ATOM	3155	C	GLY	D	69	52.580	30.012	43.952	1.00	23.05	C
ATOM	3156	O	GLY	D	69	52.270	30.941	44.691	1.00	24.04	O
ATOM	3157	N	LEU	D	70	51.883	29.667	42.870	1.00	22.75	N
ATOM	3158	CA	LEU	D	70	50.768	30.474	42.415	1.00	23.31	C
ATOM	3159	C	LEU	D	70	49.618	30.380	43.412	1.00	21.85	O
ATOM	3160	O	LEU	D	70	49.170	29.262	43.689	1.00	23.27	C
ATOM	3161	CB	LEU	D	70	50.307	29.902	41.114	1.00	22.88	C
ATOM	3162	CG	LEU	D	70	49.652	30.850	40.145	1.00	22.31	C
ATOM	3163	CD1	LEU	D	70	49.073	29.925	39.088	1.00	24.98	C
ATOM	3164	CD2	LEU	D	70	48.576	31.722	40.710	1.00	21.90	N
ATOM	3165	N	SER	D	71	49.143	31.526	43.918	1.00	19.05	C
ATOM	3166	CA	SER	D	71	48.132	31.561	44.977	1.00	16.36	C
ATOM	3167	C	SER	D	71	47.008	32.518	44.667	1.00	15.90	O
ATOM	3168	O	SER	D	71	47.262	33.701	44.521	1.00	18.19	C
ATOM	3169	CB	SER	D	71	48.747	32.015	46.298	1.00	15.26	O
ATOM	3170	OG	SER	D	71	47.822	32.217	47.360	1.00	16.34	N
ATOM	3171	N	ASN	D	72	45.757	32.053	44.598	1.00	17.24	C
ATOM	3172	CA	ASN	D	72	44.604	32.871	44.335	1.00	14.30	C
ATOM	3173	C	ASN	D	72	44.451	33.836	45.493	1.00	16.33	O
ATOM	3174	O	ASN	D	72	44.170	35.023	45.286	1.00	16.94	C
ATOM	3175	CB	ASN	D	72	43.399	31.967	44.208	1.00	14.51	C
ATOM	3176	CG	ASN	D	72	43.311	31.102	42.953	1.00	14.36	O
ATOM	3177	OD1	ASN	D	72	44.170	31.156	42.089	1.00	15.41	N
ATOM	3178	ND2	ASN	D	72	42.291	30.261	42.779	1.00	14.10	C
ATOM	3179	N	TYR	D	73	44.711	33.348	46.720	1.00	16.70	C
ATOM	3180	CA	TYR	D	73	44.709	34.222	47.893	1.00	17.86	O
ATOM	3181	C	TYR	D	73	45.580	35.466	47.698	1.00	17.22	N
ATOM	3182	O	TYR	D	73	45.047	36.559	47.813	1.00	19.51	C
ATOM	3183	CB	TYR	D	73	45.171	33.479	49.182	1.00	15.83	C
ATOM	3184	CG	TYR	D	73	44.962	34.331	50.421	1.00	11.11	C
ATOM	3185	CD1	TYR	D	73	43.755	34.297	51.064	1.00	13.95	C
ATOM	3186	CD2	TYR	D	73	45.932	35.212	50.823	1.00	14.63	C
ATOM	3187	CE1	TYR	D	73	43.474	35.184	52.080	1.00	15.34	C

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FIGURE 8A-64

ATOM	3188	CE2	TYR	D	73	45.663	36.140	51.814	1.00	15.34		C
ATOM	3189	CZ	TYR	D	73	44.430	36.108	52.407	1.00	16.30		O
ATOM	3190	OH	TYR	D	73	44.123	37.051	53.334	1.00	22.01		N
ATOM	3191	N	SER	D	74	46.888	35.357	47.402	1.00	18.57		C
ATOM	3192	CA	SER	D	74	47.786	36.498	47.221	1.00	17.90		C
ATOM	3193	C	SER	D	74	47.420	37.417	46.121	1.00	16.44		O
ATOM	3194	O	SER	D	74	47.636	38.600	46.291	1.00	18.01		C
ATOM	3195	CB	SER	D	74	49.180	36.125	46.829	1.00	18.93		N
ATOM	3196	OG	SER	D	74	49.623	35.176	47.760	1.00	25.77		C
ATOM	3197	N	ILE	D	75	46.890	36.866	45.027	1.00	16.68		O
ATOM	3198	CA	ILE	D	75	46.470	37.645	43.893	1.00	16.88		C
ATOM	3199	C	ILE	D	75	45.256	38.493	44.244	1.00	16.78		C
ATOM	3200	O	ILE	D	75	45.237	39.693	43.968	1.00	20.42		C
ATOM	3201	CB	ILE	D	75	46.184	36.709	42.711	1.00	16.41		N
ATOM	3202	CG1	ILE	D	75	47.380	35.898	42.295	1.00	16.78		C
ATOM	3203	CG2	ILE	D	75	45.861	37.615	41.567	1.00	16.46		O
ATOM	3204	CD1	ILE	D	75	47.146	34.967	41.097	1.00	19.66		C
ATOM	3205	N	ILE	D	76	44.230	37.936	44.901	1.00	18.21		C
ATOM	3206	CA	ILE	D	76	43.023	38.678	45.220	1.00	15.41		C
ATOM	3207	C	ILE	D	76	43.340	39.669	46.286	1.00	17.60		N
ATOM	3208	O	ILE	D	76	42.870	40.796	46.215	1.00	20.17		C
ATOM	3209	CB	ILE	D	76	41.941	37.743	45.711	1.00	16.42		O
ATOM	3210	CG1	ILE	D	76	41.615	36.789	44.588	1.00	14.92		C
ATOM	3211	CG2	ILE	D	76	40.696	38.481	46.200	1.00	11.21		C
ATOM	3212	CD1	ILE	D	76	40.745	35.613	45.055	1.00	13.69		C
ATOM	3213	N	ASP	D	77	44.162	39.271	47.248	1.00	19.35		N
ATOM	3214	CA	ASP	D	77	44.561	40.150	48.321	1.00	21.77		C
ATOM	3215	C	ASP	D	77	45.248	41.436	47.858	1.00	22.56		O
ATOM	3216	O	ASP	D	77	44.924	42.515	48.376	1.00	22.07		C
ATOM	3217	CB	ASP	D	77	45.433	39.385	49.282	1.00	24.17		C
ATOM	3218	CG	ASP	D	77	45.713	40.148	50.571	1.00	28.55		C
ATOM	3219	OD1	ASP	D	77	44.842	40.889	51.067	1.00	33.63		N
ATOM	3220	OD2	ASP	D	77	46.822	39.988	51.073	1.00	28.53		C
ATOM	3221	N	LYS	D	78	46.139	41.344	46.851	1.00	22.27		O
ATOM	3222	CA	LYS	D	78	46.692	42.534	46.222	1.00	21.32		C
ATOM	3223	C	LYS	D	78	45.654	43.318	45.471	1.00	19.56		C
ATOM	3224	O	LYS	D	78	45.786	44.524	45.417	1.00	22.75		O
ATOM	3225	CB	LYS	D	78	47.807	42.270	45.230	1.00	23.87		C
ATOM	3226	CG	LYS	D	78	49.036	41.600	45.795	1.00	30.71		C
ATOM	3227	CD	LYS	D	78	50.269	41.917	44.947	1.00	37.30		C
ATOM	3228	CE	LYS	D	78	51.317	40.799	45.004	1.00	40.34		N
ATOM	3229	NZ	LYS	D	78	50.843	39.671	44.214	1.00	44.85		N
ATOM	3230	N	LEU	D	79	44.634	42.714	44.882	1.00	18.00		C
ATOM	3231	CA	LEU	D	79	43.570	43.462	44.247	1.00	16.42		O
ATOM	3232	C	LEU	D	79	42.696	44.124	45.273	1.00	18.98		C
ATOM	3233	O	LEU	D	79	42.215	45.218	45.035	1.00	21.86		C
ATOM	3234	CB	LEU	D	79	42.687	42.543	43.451	1.00	13.71		C
ATOM	3235	CG	LEU	D	79	43.383	41.746	42.358	1.00	13.81		N
ATOM	3236	CD1	LEU	D	79	42.294	41.091	41.522	1.00	14.16		C
ATOM	3237	CD2	LEU	D	79	44.240	42.627	41.462	1.00	11.49		C
ATOM	3238	N	VAL	D	80	42.438	43.524	46.430	1.00	19.01		C
ATOM	3239	CA	VAL	D	80	41.624	44.124	47.462	1.00	20.11		N
ATOM	3240	C	VAL	D	80	42.369	45.343	47.920	1.00	21.57		C
ATOM	3241	O	VAL	D	80	41.759	46.389	47.987	1.00	25.14		O
ATOM	3242	CB	VAL	D	80	41.480	43.093	48.603	1.00	22.94		C
ATOM	3243	CG1	VAL	D	80	40.920	43.647	49.896	1.00	25.85		C
ATOM	3244	CG2	VAL	D	80	40.511	42.003	48.246	1.00	20.39		N
ATOM	3245	N	ASN	D	81	43.678	45.313	48.167	1.00	24.08		C
ATOM	3246	CA	ASN	D	81	44.375	46.498	48.626	1.00	23.59		C
ATOM	3247	C	ASN	D	81	44.363	47.632	47.620	1.00	26.17		C

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FIGURE 8A-65

ATOM	3248	O	ASN	D	81	44.334	48.756	48.114	1.00	28.26	O
ATOM	3249	CB	ASN	D	81	45.761	46.180	49.097	1.00	21.14	C
ATOM	3250	CG	ASN	D	81	45.684	45.257	50.278	1.00	23.73	C
ATOM	3251	OD1	ASN	D	81	44.871	45.422	51.175	1.00	31.16	O
ATOM	3252	ND2	ASN	D	81	46.490	44.231	50.357	1.00	25.26	N
ATOM	3253	N	ILE	D	82	44.340	47.414	46.280	1.00	25.02	N
ATOM	3254	CA	ILE	D	82	44.088	48.469	45.268	1.00	25.82	C
ATOM	3255	C	ILE	D	82	42.671	49.103	45.287	1.00	25.89	C
ATOM	3256	O	ILE	D	82	42.512	50.323	45.196	1.00	25.87	O
ATOM	3257	CB	ILE	D	82	44.444	48.002	43.847	1.00	23.39	C
ATOM	3258	CG1	ILE	D	82	45.885	47.557	43.751	1.00	25.26	C
ATOM	3259	CG2	ILE	D	82	44.317	49.150	42.894	1.00	23.94	C
ATOM	3260	CD1	ILE	D	82	46.185	46.717	42.500	1.00	24.24	C
ATOM	3261	N	VAL	D	83	41.595	48.324	45.443	1.00	27.50	N
ATOM	3262	CA	VAL	D	83	40.240	48.859	45.486	1.00	27.69	C
ATOM	3263	C	VAL	D	83	40.017	49.556	46.841	1.00	30.42	C
ATOM	3264	O	VAL	D	83	39.190	50.454	46.938	1.00	29.44	O
ATOM	3265	CB	VAL	D	83	39.230	47.758	45.201	1.00	23.07	C
ATOM	3266	CG1	VAL	D	83	37.910	48.384	44.868	1.00	24.95	C
ATOM	3267	CG2	VAL	D	83	39.634	47.000	43.979	1.00	23.59	C
ATOM	3268	N	ASP	D	84	40.772	49.192	47.892	1.00	32.89	N
ATOM	3269	CA	ASP	D	84	40.753	49.840	49.206	1.00	35.85	C
ATOM	3270	C	ASP	D	84	41.361	51.238	49.084	1.00	35.75	C
ATOM	3271	O	ASP	D	84	40.779	52.212	49.557	1.00	35.62	O
ATOM	3272	CB	ASP	D	84	41.531	49.029	50.294	1.00	39.03	C
ATOM	3273	CG	ASP	D	84	40.827	48.006	51.221	1.00	41.67	C
ATOM	3274	OD1	ASP	D	84	39.593	47.858	51.172	1.00	43.23	O
ATOM	3275	OD2	ASP	D	84	41.536	47.352	52.008	1.00	43.54	O
ATOM	3276	N	ASP	D	85	42.500	51.382	48.417	1.00	35.24	N
ATOM	3277	CA	ASP	D	85	43.039	52.689	48.095	1.00	39.54	C
ATOM	3278	C	ASP	D	85	42.055	53.620	47.372	1.00	40.48	C
ATOM	3279	O	ASP	D	85	41.712	54.706	47.853	1.00	42.05	O
ATOM	3280	CB	ASP	D	85	44.343	52.540	47.287	1.00	41.18	C
ATOM	3281	CG	ASP	D	85	45.534	51.871	48.001	1.00	43.42	C
ATOM	3282	OD1	ASP	D	85	45.537	51.723	49.243	1.00	41.35	O
ATOM	3283	OD2	ASP	D	85	46.465	51.488	47.276	1.00	42.78	O
ATOM	3284	N	LEU	D	86	41.518	53.157	46.238	1.00	41.90	N
ATOM	3285	CA	LEU	D	86	40.526	53.903	45.456	1.00	39.57	C
ATOM	3286	C	LEU	D	86	39.249	54.172	46.203	1.00	38.81	C
ATOM	3287	O	LEU	D	86	38.614	55.176	45.924	1.00	40.16	O
ATOM	3288	CB	LEU	D	86	40.142	53.164	44.191	1.00	36.00	C
ATOM	3289	CG	LEU	D	86	41.234	52.732	43.251	1.00	34.91	C
ATOM	3290	CD1	LEU	D	86	40.618	52.075	42.047	1.00	33.95	C
ATOM	3291	CD2	LEU	D	86	42.006	53.907	42.858	1.00	32.40	C
ATOM	3292	N	VAL	D	87	38.840	53.303	47.125	1.00	40.82	N
ATOM	3293	CA	VAL	D	87	37.680	53.589	47.958	1.00	44.87	C
ATOM	3294	C	VAL	D	87	37.965	54.754	48.933	1.00	47.95	C
ATOM	3295	O	VAL	D	87	37.085	55.580	49.176	1.00	49.04	O
ATOM	3296	CB	VAL	D	87	37.191	52.311	48.682	1.00	42.48	C
ATOM	3297	CG1	VAL	D	87	36.094	52.685	49.647	1.00	43.30	C
ATOM	3298	CG2	VAL	D	87	36.572	51.285	47.749	1.00	39.59	C
ATOM	3299	N	GLU	D	88	39.185	54.862	49.472	1.00	51.32	N
ATOM	3300	CA	GLU	D	88	39.548	55.935	50.387	1.00	55.88	C
ATOM	3301	C	GLU	D	88	39.807	57.235	49.672	1.00	57.32	C
ATOM	3302	O	GLU	D	88	39.717	58.303	50.291	1.00	59.78	O
ATOM	3303	CB	GLU	D	88	40.786	55.627	51.225	1.00	57.84	C
ATOM	3304	CG	GLU	D	88	40.534	54.935	52.572	1.00	61.46	C
ATOM	3305	CD	GLU	D	88	41.737	54.106	53.056	1.00	65.66	C
ATOM	3306	OE1	GLU	D	88	42.872	54.610	53.000	1.00	65.91	O
ATOM	3307	OE2	GLU	D	88	41.543	52.947	53.479	1.00	68.20	O

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FIGURE 8A-66

ATOM	3308	N	CYS	D	89	40.147	57.130	48.382	1.00	57.61	N
ATOM	3309	CA	CYS	D	89	40.273	58.307	47.528	1.00	58.46	C
ATOM	3310	C	CYS	D	89	38.895	58.970	47.344	1.00	58.39	C
ATOM	3311	O	CYS	D	89	38.791	60.197	47.378	1.00	58.21	O
ATOM	3312	CB	CYS	D	89	40.931	57.880	46.221	1.00	57.54	C
ATOM	3313	SG	CYS	D	89	41.341	59.181	45.038	1.00	58.90	S
ATOM	3314	N	VAL	D	90	37.809	58.179	47.271	1.00	58.70	N
ATOM	3315	CA	VAL	D	90	36.453	58.684	47.150	1.00	59.63	C
ATOM	3316	C	VAL	D	90	35.871	59.210	48.484	1.00	61.73	C
ATOM	3317	O	VAL	D	90	34.680	59.004	48.763	1.00	62.80	O
ATOM	3318	CB	VAL	D	90	35.602	57.544	46.539	1.00	58.55	C
ATOM	3319	N	SER	D	104	20.665	52.244	45.909	1.00	56.19	N
ATOM	3320	CA	SER	D	104	21.629	51.156	45.958	1.00	53.75	C
ATOM	3321	C	SER	D	104	21.476	50.204	44.750	1.00	51.69	C
ATOM	3322	O	SER	D	104	20.519	50.365	43.954	1.00	53.93	O
ATOM	3323	CB	SER	D	104	21.454	50.421	47.297	1.00	55.38	C
ATOM	3324	OG	SER	D	104	22.506	49.503	47.610	1.00	56.37	O
ATOM	3325	N	PRO	D	105	22.446	49.277	44.526	1.00	45.68	N
ATOM	3326	CA	PRO	D	105	22.366	48.292	43.470	1.00	41.30	C
ATOM	3327	C	PRO	D	105	22.138	46.887	43.955	1.00	37.99	C
ATOM	3328	O	PRO	D	105	22.529	46.478	45.049	1.00	38.93	O
ATOM	3329	CB	PRO	D	105	23.661	48.481	42.741	1.00	40.55	C
ATOM	3330	CG	PRO	D	105	24.631	48.664	43.862	1.00	42.00	C
ATOM	3331	CD	PRO	D	105	23.856	49.476	44.863	1.00	42.72	C
ATOM	3332	N	GLU	D	106	21.459	46.177	43.075	1.00	33.70	N
ATOM	3333	CA	GLU	D	106	20.971	44.880	43.417	1.00	32.02	C
ATOM	3334	C	GLU	D	106	21.976	43.812	43.085	1.00	32.36	C
ATOM	3335	O	GLU	D	106	22.715	43.942	42.111	1.00	32.37	O
ATOM	3336	CB	GLU	D	106	19.734	44.553	42.624	1.00	32.57	C
ATOM	3337	N	PRO	D	107	22.006	42.732	43.886	1.00	32.45	N
ATOM	3338	CA	PRO	D	107	22.855	41.549	43.686	1.00	31.86	C
ATOM	3339	C	PRO	D	107	22.724	40.845	42.340	1.00	29.45	C
ATOM	3340	O	PRO	D	107	21.623	40.491	41.911	1.00	29.62	O
ATOM	3341	CB	PRO	D	107	22.403	40.614	44.801	1.00	32.83	C
ATOM	3342	CG	PRO	D	107	22.040	41.574	45.904	1.00	34.59	C
ATOM	3343	CD	PRO	D	107	21.299	42.658	45.165	1.00	31.98	C
ATOM	3344	N	ARG	D	108	23.893	40.580	41.745	1.00	27.04	N
ATOM	3345	CA	ARG	D	108	23.966	39.882	40.479	1.00	24.37	C
ATOM	3346	C	ARG	D	108	25.090	38.834	40.442	1.00	22.83	C
ATOM	3347	O	ARG	D	108	26.084	39.002	41.124	1.00	21.26	O
ATOM	3348	CB	ARG	D	108	24.090	40.981	39.431	1.00	27.20	C
ATOM	3349	CG	ARG	D	108	23.924	40.490	38.015	1.00	32.52	C
ATOM	3350	CD	ARG	D	108	23.488	41.587	37.051	1.00	35.27	C
ATOM	3351	NE	ARG	D	108	23.846	41.160	35.712	1.00	38.19	N
ATOM	3352	CZ	ARG	D	108	23.536	41.872	34.627	1.00	38.97	C
ATOM	3353	NH1	ARG	D	108	22.798	43.008	34.720	1.00	34.64	N
ATOM	3354	NH2	ARG	D	108	23.995	41.398	33.454	1.00	39.61	N
ATOM	3355	N	LEU	D	109	24.984	37.734	39.681	1.00	21.95	N
ATOM	3356	CA	LEU	D	109	25.996	36.697	39.565	1.00	20.44	C
ATOM	3357	C	LEU	D	109	26.760	36.756	38.265	1.00	18.72	C
ATOM	3358	O	LEU	D	109	26.191	36.725	37.175	1.00	19.50	O
ATOM	3359	CB	LEU	D	109	25.392	35.304	39.657	1.00	21.02	C
ATOM	3360	CG	LEU	D	109	24.434	34.885	40.779	1.00	23.43	C
ATOM	3361	CD1	LEU	D	109	24.170	33.404	40.648	1.00	24.08	C
ATOM	3362	CD2	LEU	D	109	24.939	35.187	42.193	1.00	25.25	C
ATOM	3363	N	PHE	D	110	28.080	36.753	38.437	1.00	17.94	N
ATOM	3364	CA	PHE	D	110	29.031	36.804	37.333	1.00	17.25	C
ATOM	3365	C	PHE	D	110	30.013	35.649	37.346	1.00	16.87	C
ATOM	3366	O	PHE	D	110	30.417	35.198	38.404	1.00	19.49	O
ATOM	3367	CB	PHE	D	110	29.848	38.070	37.366	1.00	16.08	C

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FIGURE 8A-67

ATOM	3368	CG	PHE	D	110	28.993	39.305	37.265	1.00	18.38	C
ATOM	3369	CD1	PHE	D	110	28.573	39.743	36.029	1.00	19.11	C
ATOM	3370	CD2	PHE	D	110	28.633	39.977	38.408	1.00	16.78	C
ATOM	3371	CE1	PHE	D	110	27.802	40.874	35.946	1.00	16.73	C
ATOM	3372	CE2	PHE	D	110	27.850	41.103	38.321	1.00	18.17	C
ATOM	3373	CZ	PHE	D	110	27.445	41.553	37.081	1.00	21.53	C
ATOM	3374	N	THR	D	111	30.425	35.107	36.216	1.00	15.24	N
ATOM	3375	CA	THR	D	111	31.539	34.192	36.176	1.00	14.72	C
ATOM	3376	C	THR	D	111	32.811	34.994	36.443	1.00	12.40	C
ATOM	3377	O	THR	D	111	32.752	36.218	36.400	1.00	13.27	O
ATOM	3378	CB	THR	D	111	31.579	33.435	34.828	1.00	17.12	C
ATOM	3379	OG1	THR	D	111	31.630	34.415	33.809	1.00	17.68	O
ATOM	3380	CG2	THR	D	111	30.451	32.446	34.621	1.00	14.81	C
ATOM	3381	N	PRO	D	112	33.974	34.412	36.757	1.00	12.31	N
ATOM	3382	CA	PRO	D	112	35.219	35.126	36.935	1.00	11.10	C
ATOM	3383	C	PRO	D	112	35.594	36.046	35.783	1.00	14.02	C
ATOM	3384	O	PRO	D	112	35.884	37.215	36.011	1.00	13.17	O
ATOM	3385	CB	PRO	D	112	36.189	33.965	37.074	1.00	9.39	C
ATOM	3386	CG	PRO	D	112	35.413	32.952	37.854	1.00	7.72	C
ATOM	3387	CD	PRO	D	112	34.151	32.972	37.061	1.00	11.01	C
ATOM	3388	N	GLU	D	113	35.611	35.572	34.517	1.00	16.22	N
ATOM	3389	CA	GLU	D	113	35.905	36.456	33.395	1.00	16.17	C
ATOM	3390	C	GLU	D	113	35.026	37.679	33.272	1.00	13.99	C
ATOM	3391	O	GLU	D	113	35.508	38.761	32.985	1.00	15.09	O
ATOM	3392	CB	GLU	D	113	35.913	35.703	32.092	1.00	17.91	C
ATOM	3393	CG	GLU	D	113	34.636	34.985	31.713	1.00	19.43	C
ATOM	3394	CD	GLU	D	113	34.621	34.539	30.277	1.00	22.34	C
ATOM	3395	OE1	GLU	D	113	35.652	34.599	29.608	1.00	23.91	O
ATOM	3396	OE2	GLU	D	113	33.558	34.139	29.810	1.00	24.64	O
ATOM	3397	N	GLU	D	114	33.747	37.539	33.559	1.00	14.85	N
ATOM	3398	CA	GLU	D	114	32.837	38.649	33.596	1.00	15.81	C
ATOM	3399	C	GLU	D	114	33.063	39.567	34.769	1.00	15.50	C
ATOM	3400	O	GLU	D	114	33.085	40.783	34.557	1.00	15.87	O
ATOM	3401	CB	GLU	D	114	31.402	38.208	33.707	1.00	19.13	C
ATOM	3402	CG	GLU	D	114	30.883	37.422	32.539	1.00	21.49	C
ATOM	3403	CD	GLU	D	114	29.605	36.642	32.816	1.00	24.09	C
ATOM	3404	OE1	GLU	D	114	29.017	36.697	33.897	1.00	26.51	O
ATOM	3405	OE2	GLU	D	114	29.185	35.937	31.907	1.00	29.29	O
ATOM	3406	N	PHE	D	115	33.204	39.041	35.990	1.00	13.99	N
ATOM	3407	CA	PHE	D	115	33.464	39.892	37.125	1.00	12.83	C
ATOM	3408	C	PHE	D	115	34.753	40.667	36.905	1.00	13.21	C
ATOM	3409	O	PHE	D	115	34.827	41.855	37.193	1.00	14.99	O
ATOM	3410	CB	PHE	D	115	33.650	39.018	38.359	1.00	10.89	C
ATOM	3411	CG	PHE	D	115	33.982	39.867	39.569	1.00	11.83	C
ATOM	3412	CD1	PHE	D	115	32.951	40.361	40.344	1.00	12.60	C
ATOM	3413	CD2	PHE	D	115	35.296	40.133	39.917	1.00	14.96	C
ATOM	3414	CE1	PHE	D	115	33.251	41.093	41.480	1.00	12.59	C
ATOM	3415	CE2	PHE	D	115	35.605	40.892	41.033	1.00	13.04	C
ATOM	3416	CZ	PHE	D	115	34.560	41.373	41.810	1.00	14.57	C
ATOM	3417	N	PHE	D	116	35.833	40.025	36.477	1.00	15.07	N
ATOM	3418	CA	PHE	D	116	37.102	40.718	36.297	1.00	13.94	C
ATOM	3419	C	PHE	D	116	37.181	41.563	35.036	1.00	15.79	C
ATOM	3420	O	PHE	D	116	38.014	42.455	34.965	1.00	16.79	O
ATOM	3421	CB	PHE	D	116	38.273	39.775	36.373	1.00	13.55	C
ATOM	3422	CG	PHE	D	116	38.548	39.261	37.759	1.00	10.27	C
ATOM	3423	CD1	PHE	D	116	39.105	40.100	38.692	1.00	12.82	C
ATOM	3424	CD2	PHE	D	116	38.143	37.990	38.132	1.00	11.47	C
ATOM	3425	CE1	PHE	D	116	39.169	39.689	40.025	1.00	14.46	C
ATOM	3426	CE2	PHE	D	116	38.216	37.584	39.457	1.00	10.67	C
ATOM	3427	CZ	PHE	D	116	38.709	38.439	40.407	1.00	11.80	C

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FIGURE 8A-68

ATOM	3428	N	ARG	D	117	36.361	41.405	34.011	1.00	16.57	N
ATOM	3429	CA	ARG	D	117	36.293	42.421	32.990	1.00	20.64	C
ATOM	3430	C	ARG	D	117	35.668	43.700	33.548	1.00	22.51	C
ATOM	3431	O	ARG	D	117	36.089	44.803	33.174	1.00	23.89	O
ATOM	3432	CB	ARG	D	117	35.446	41.879	31.860	1.00	26.52	C
ATOM	3433	CG	ARG	D	117	35.518	42.709	30.598	1.00	31.58	C
ATOM	3434	CD	ARG	D	117	34.496	42.146	29.640	1.00	35.05	C
ATOM	3435	NE	ARG	D	117	34.394	43.021	28.483	1.00	38.58	N
ATOM	3436	CZ	ARG	D	117	33.828	42.656	27.326	1.00	37.56	C
ATOM	3437	NH1	ARG	D	117	33.169	41.506	27.170	1.00	33.95	N
ATOM	3438	NH2	ARG	D	117	34.002	43.473	26.286	1.00	37.95	N
ATOM	3439	N	ILE	D	118	34.656	43.594	34.445	1.00	22.03	N
ATOM	3440	CA	ILE	D	118	34.052	44.753	35.121	1.00	19.63	C
ATOM	3441	C	ILE	D	118	35.047	45.368	36.086	1.00	19.88	C
ATOM	3442	O	ILE	D	118	35.183	46.586	36.085	1.00	23.21	O
ATOM	3443	CB	ILE	D	118	32.781	44.357	35.874	1.00	20.68	C
ATOM	3444	CG1	ILE	D	118	31.691	43.843	34.951	1.00	19.48	C
ATOM	3445	CG2	ILE	D	118	32.255	45.562	36.619	1.00	20.52	C
ATOM	3446	CD1	ILE	D	118	30.567	43.143	35.727	1.00	18.63	C
ATOM	3447	N	PHE	D	119	35.741	44.577	36.908	1.00	16.07	N
ATOM	3448	CA	PHE	D	119	36.853	45.059	37.683	1.00	15.72	C
ATOM	3449	C	PHE	D	119	37.853	45.894	36.880	1.00	17.75	C
ATOM	3450	O	PHE	D	119	38.208	47.006	37.267	1.00	20.22	O
ATOM	3451	CB	PHE	D	119	37.545	43.866	38.359	1.00	12.02	C
ATOM	3452	CG	PHE	D	119	38.822	44.222	39.100	1.00	13.89	C
ATOM	3453	CD1	PHE	D	119	38.760	44.766	40.389	1.00	14.47	C
ATOM	3454	CD2	PHE	D	119	40.057	44.030	38.492	1.00	10.48	C
ATOM	3455	CE1	PHE	D	119	39.944	45.148	41.032	1.00	13.14	C
ATOM	3456	CE2	PHE	D	119	41.219	44.387	39.149	1.00	10.95	C
ATOM	3457	CZ	PHE	D	119	41.163	44.965	40.405	1.00	10.47	C
ATOM	3458	N	ASN	D	120	38.349	45.343	35.779	1.00	18.18	N
ATOM	3459	CA	ASN	D	120	39.325	45.994	34.955	1.00	18.15	C
ATOM	3460	C	ASN	D	120	38.709	47.263	34.387	1.00	20.79	C
ATOM	3461	O	ASN	D	120	39.348	48.303	34.408	1.00	22.36	O
ATOM	3462	CB	ASN	D	120	39.805	45.078	33.812	1.00	18.05	C
ATOM	3463	CG	ASN	D	120	40.849	44.026	34.137	1.00	17.71	C
ATOM	3464	OD1	ASN	D	120	41.770	44.210	34.918	1.00	21.36	O
ATOM	3465	ND2	ASN	D	120	40.765	42.860	33.538	1.00	17.03	N
ATOM	3466	N	ARG	D	121	37.463	47.256	33.941	1.00	22.71	N
ATOM	3467	CA	ARG	D	121	36.824	48.438	33.431	1.00	24.59	C
ATOM	3468	C	ARG	D	121	36.703	49.523	34.494	1.00	27.41	C
ATOM	3469	O	ARG	D	121	36.971	50.683	34.192	1.00	30.49	O
ATOM	3470	CB	ARG	D	121	35.468	47.993	32.953	1.00	26.42	C
ATOM	3471	CG	ARG	D	121	34.608	49.156	32.549	1.00	33.46	C
ATOM	3472	CD	ARG	D	121	34.760	49.641	31.105	1.00	37.32	C
ATOM	3473	NE	ARG	D	121	34.149	50.962	30.882	1.00	39.99	N
ATOM	3474	CZ	ARG	D	121	32.836	51.217	31.020	1.00	39.01	C
ATOM	3475	NH1	ARG	D	121	31.955	50.306	31.426	1.00	37.27	N
ATOM	3476	NH2	ARG	D	121	32.392	52.439	30.747	1.00	40.47	N
ATOM	3477	N	SER	D	122	36.364	49.186	35.754	1.00	28.07	N
ATOM	3478	CA	SER	D	122	36.147	50.153	36.820	1.00	24.66	C
ATOM	3479	C	SER	D	122	37.455	50.758	37.250	1.00	25.38	C
ATOM	3480	O	SER	D	122	37.536	51.971	37.401	1.00	24.85	O
ATOM	3481	CB	SER	D	122	35.452	49.505	37.983	1.00	20.76	C
ATOM	3482	OG	SER	D	122	34.236	48.886	37.591	1.00	19.10	O
ATOM	3483	N	ILE	D	123	38.513	49.954	37.389	1.00	28.58	N
ATOM	3484	CA	ILE	D	123	39.853	50.468	37.718	1.00	31.03	C
ATOM	3485	C	ILE	D	123	40.396	51.464	36.684	1.00	33.54	C
ATOM	3486	O	ILE	D	123	40.998	52.471	37.040	1.00	33.54	O
ATOM	3487	CB	ILE	D	123	40.821	49.267	38.041	1.00	31.69	C

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FIGURE 8A-69

ATOM	3488	CG1	ILE	D	123	40.899	48.877	39.544	1.00	30.91	C
ATOM	3489	CG2	ILE	D	123	42.262	49.504	37.583	1.00	31.27	C
ATOM	3490	CD1	ILE	D	123	39.609	48.826	40.377	1.00	31.19	C
ATOM	3491	N	ASP	D	124	40.123	51.244	35.395	1.00	36.80	N
ATOM	3492	CA	ASP	D	124	40.562	52.125	34.333	1.00	38.72	C
ATOM	3493	C	ASP	D	124	39.846	53.455	34.353	1.00	39.18	C
ATOM	3494	O	ASP	D	124	40.487	54.491	34.186	1.00	39.94	O
ATOM	3495	CB	ASP	D	124	40.383	51.461	32.981	1.00	42.50	C
ATOM	3496	CG	ASP	D	124	40.847	52.342	31.828	1.00	47.69	C
ATOM	3497	OD1	ASP	D	124	42.058	52.554	31.646	1.00	50.62	O
ATOM	3498	OD2	ASP	D	124	39.972	52.837	31.116	1.00	51.18	O
ATOM	3499	N	ALA	D	125	38.538	53.440	34.590	1.00	39.43	N
ATOM	3500	CA	ALA	D	125	37.731	54.649	34.586	1.00	41.04	C
ATOM	3501	C	ALA	D	125	38.028	55.640	35.712	1.00	44.24	C
ATOM	3502	O	ALA	D	125	37.580	56.792	35.729	1.00	46.63	O
ATOM	3503	CB	ALA	D	125	36.289	54.232	34.688	1.00	37.89	C
ATOM	3504	N	PHE	D	126	38.795	55.189	36.693	1.00	47.55	N
ATOM	3505	CA	PHE	D	126	39.342	56.063	37.709	1.00	52.08	C
ATOM	3506	C	PHE	D	126	40.409	57.058	37.208	1.00	55.06	C
ATOM	3507	O	PHE	D	126	40.531	58.167	37.751	1.00	57.33	O
ATOM	3508	CB	PHE	D	126	39.877	55.182	38.838	1.00	51.90	C
ATOM	3509	CG	PHE	D	126	39.154	55.489	40.124	1.00	50.92	C
ATOM	3510	CD1	PHE	D	126	39.155	56.780	40.620	1.00	52.88	C
ATOM	3511	CD2	PHE	D	126	38.437	54.505	40.745	1.00	50.11	C
ATOM	3512	CE1	PHE	D	126	38.390	57.105	41.721	1.00	54.34	C
ATOM	3513	CE2	PHE	D	126	37.688	54.827	41.851	1.00	52.08	C
ATOM	3514	CZ	PHE	D	126	37.653	56.117	42.336	1.00	53.64	C
ATOM	3515	N	LYS	D	127	41.187	56.667	36.177	1.00	56.75	N
ATOM	3516	CA	LYS	D	127	42.055	57.566	35.420	1.00	57.29	C
ATOM	3517	C	LYS	D	127	41.257	58.229	34.273	1.00	58.91	C
ATOM	3518	O	LYS	D	127	41.376	57.826	33.098	1.00	60.03	O
ATOM	3519	CB	LYS	D	127	43.225	56.735	34.882	1.00	56.61	C
TER	3521		LYS	D	127						
HETATM	3522	CA	CA		1021	34.563	32.796	27.927	1.00	28.47	CA
HETATM	3523	CA	CA		1022	29.874	41.216	51.866	1.00	42.93	CA
HETATM	3524	CA	CA		1023	46.453	8.630	31.415	1.00	34.99	CA
HETATM	3525	OH2	1PE		1	18.016	39.096	31.870	1.00	54.04	O
HETATM	3526	C12	1PE		1	19.233	39.467	31.241	1.00	52.50	C
HETATM	3527	C22	1PE		1	20.344	39.764	32.285	1.00	52.87	C
HETATM	3528	OH3	1PE		1	21.455	40.455	31.657	1.00	50.81	O
HETATM	3529	C13	1PE		1	21.887	42.392	30.182	1.00	41.29	C
HETATM	3530	C23	1PE		1	20.971	41.737	31.213	1.00	45.45	C
HETATM	3531	OH4	1PE		1	23.085	42.870	30.757	1.00	37.80	O
HETATM	3532	C14	1PE		1	24.265	44.731	31.534	1.00	39.00	C
HETATM	3533	C24	1PE		1	22.866	44.120	31.391	1.00	35.49	C
HETATM	3534	OH5	1PE		1	25.158	43.676	31.917	1.00	39.07	O
HETATM	3535	C15	1PE		1	27.396	42.942	31.976	1.00	36.51	C
HETATM	3536	C25	1PE		1	26.476	44.138	32.222	1.00	37.63	C
HETATM	3537	OH6	1PE		1	26.797	41.817	32.602	1.00	37.94	O
HETATM	3538	C16	1PE		1	28.795	40.537	32.878	1.00	44.86	C
HETATM	3539	C26	1PE		1	27.405	40.589	32.251	1.00	38.90	C
HETATM	3540	OH7	1PE		1	29.817	40.999	31.987	1.00	53.59	O
HETATM	3541	O	HOH		1024	36.890	32.430	27.721	1.00	24.58	O
HETATM	3542	O	HOH		1025	35.049	30.934	29.322	1.00	27.97	O
HETATM	3543	O	HOH		1026	31.347	42.865	52.839	1.00	31.45	O
HETATM	3544	O	HOH		1027	44.819	10.251	32.056	1.00	31.08	O
HETATM	3545	O	HOH		1028	47.508	7.695	33.365	1.00	35.15	O
HETATM	3546	O	HOH		1029	48.695	9.256	30.957	1.00	29.22	O
HETATM	3547	O	HOH		1105	33.704	13.935	20.986	1.00	32.21	O
HETATM	3548	O	HOH		1106	22.707	17.800	13.006	1.00	51.74	O

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FIGURE 8A-70

HETATM	3549	O	HOH	1107	25.589	22.952	23.068	1.00 38.86
HETATM	3550	O	HOH	1108	20.410	17.104	15.299	1.00 29.07
HETATM	3551	O	HOH	1109	26.763	8.355	29.315	1.00 19.21
HETATM	3552	O	HOH	1110	25.744	13.365	30.461	1.00 32.06
HETATM	3553	O	HOH	1111	27.532	6.721	32.848	1.00 38.65
HETATM	3554	O	HOH	1112	18.245	18.266	16.629	1.00 28.39
HETATM	3555	O	HOH	1113	23.260	14.366	29.164	1.00 21.00
HETATM	3556	O	HOH	1114	15.116	22.225	22.815	1.00 19.32
HETATM	3557	O	HOH	1115	15.033	21.355	35.696	1.00 38.95
HETATM	3558	O	HOH	1116	20.651	6.306	35.427	1.00 25.08
HETATM	3559	O	HOH	1117	15.267	18.912	37.475	1.00 41.62
HETATM	3560	O	HOH	1118	13.693	14.872	13.312	1.00 29.91
HETATM	3561	O	HOH	1119	10.257	20.310	28.411	1.00 19.75
HETATM	3562	O	HOH	1120	17.034	0.246	35.599	1.00 32.81
HETATM	3563	O	HOH	1121	6.051	17.933	31.202	1.00 21.61
HETATM	3564	O	HOH	1122	4.997	14.576	24.993	1.00 33.94
HETATM	3565	O	HOH	1123	0.916	19.643	30.618	1.00 37.91
HETATM	3566	O	HOH	1124	5.906	11.136	30.408	1.00 46.39
HETATM	3567	O	HOH	1125	6.559	5.604	30.508	1.00 37.39
HETATM	3568	O	HOH	1126	8.033	4.439	28.006	1.00 43.67
HETATM	3569	O	HOH	1127	5.753	3.756	33.445	1.00 43.48
HETATM	3570	O	HOH	1128	44.059	26.360	36.277	1.00 22.42
HETATM	3571	O	HOH	1129	34.421	31.639	20.635	1.00 57.58
HETATM	3572	O	HOH	1130	50.215	13.426	34.211	1.00 31.74
HETATM	3573	O	HOH	1132	22.455	45.496	39.519	1.00 46.16
HETATM	3574	O	HOH	1133	13.246	35.686	8.764	1.00 63.66
HETATM	3575	O	HOH	1134	34.029	21.538	54.154	1.00 48.71
HETATM	3576	O	HOH	1135	46.505	41.139	53.506	1.00 25.80
HETATM	3577	O	HOH	1136	14.868	40.514	7.810	1.00 46.95
HETATM	3578	O	HOH	1138	37.977	45.274	53.726	1.00 41.75
HETATM	3579	O	HOH	1139	10.511	41.610	30.508	1.00 54.06
HETATM	3580	O	HOH	1140	21.928	44.651	36.769	1.00 27.65
HETATM	3581	O	HOH	1141	9.657	38.390	31.085	1.00 36.52
HETATM	3582	O	HOH	1142	35.556	55.905	31.455	1.00 33.05
HETATM	3583	O	HOH	1143	52.337	31.433	47.975	1.00 42.15
HETATM	3584	O	HOH	1144	32.915	38.699	23.494	1.00 40.84
HETATM	3585	O	HOH	1145	29.548	21.469	24.434	1.00 44.50
HETATM	3586	O	HOH	1146	26.181	34.331	29.823	1.00 34.71
HETATM	3587	O	HOH	1147	39.069	5.943	33.085	1.00 53.70
HETATM	3588	O	HOH	1148	34.970	24.222	52.427	1.00 40.12
HETATM	3589	O	HOH	1149	59.825	24.478	48.580	1.00 40.98
HETATM	3590	O	HOH	1150	28.412	33.531	47.673	1.00 44.44
HETATM	3591	O	HOH	1151	25.454	33.933	32.960	1.00 35.88
HETATM	3592	O	HOH	1152	41.875	59.115	53.350	1.00 51.54
HETATM	3593	O	HOH	1153	45.977	17.661	29.654	1.00 48.44
HETATM	3594	O	HOH	1154	16.374	19.854	15.198	1.00 26.92
HETATM	3595	O	HOH	1156	2.909	45.550	9.710	1.00 33.50
HETATM	3596	O	HOH	1157	27.955	42.970	52.054	1.00 42.09
HETATM	3597	O	HOH	1158	18.671	28.692	31.947	1.00 31.92
HETATM	3598	O	HOH	1160	31.097	11.069	39.837	1.00 22.54
HETATM	3599	O	HOH	1161	24.551	47.693	13.911	1.00 39.92
HETATM	3600	O	HOH	1162	19.328	46.523	39.555	1.00 49.64
HETATM	3601	O	HOH	1163	14.463	28.577	32.747	1.00 33.62
HETATM	3602	O	HOH	1164	42.334	34.141	31.684	1.00 25.02
HETATM	3603	O	HOH	1165	26.640	35.518	34.853	1.00 25.40
HETATM	3604	O	HOH	1166	41.719	26.191	52.537	1.00 54.23
HETATM	3605	O	HOH	1167	11.799	43.370	8.564	1.00 42.64
HETATM	3606	O	HOH	1169	39.695	23.691	29.775	1.00 46.55
HETATM	3607	O	HOH	1170	25.519	-10.203	13.390	1.00 29.39
HETATM	3608	O	HOH	1172	15.639	30.378	9.410	1.00 35.98

FIGURE 8A-71

HETATM	3609	O	HOH	1173	26.042	53.508	19.228	1.00 35.35
HETATM	3610	O	HOH	1174	16.723	43.317	9.437	1.00 70.54
HETATM	3611	O	HOH	1175	11.039	27.202	31.989	1.00 35.23
HETATM	3612	O	HOH	1176	26.492	54.880	14.660	1.00 45.35
HETATM	3613	O	HOH	1177	48.739	5.603	40.080	1.00 46.72
HETATM	3614	O	HOH	1179	38.452	10.611	56.410	1.00 33.18
HETATM	3615	O	HOH	1180	25.173	41.020	50.981	1.00 37.80
HETATM	3616	O	HOH	1181	26.009	21.500	26.306	1.00 37.33
HETATM	3617	O	HOH	1185	32.901	61.354	32.974	1.00 47.36
HETATM	3618	O	HOH	1186	49.199	44.404	48.616	1.00 55.72
HETATM	3619	O	HOH	1187	28.401	31.064	46.621	1.00 25.46
HETATM	3620	O	HOH	1189	50.488	34.252	43.662	1.00 27.11
HETATM	3621	O	HOH	1190	25.015	38.231	32.413	1.00 46.20
HETATM	3622	O	HOH	1191	13.328	45.647	6.880	1.00 50.19
HETATM	3623	O	HOH	1192	9.102	28.582	30.815	1.00 28.84
HETATM	3624	O	HOH	1194	16.216	53.125	18.778	1.00 20.19
HETATM	3625	O	HOH	1195	48.924	37.778	50.511	1.00 41.81
HETATM	3626	O	HOH	1196	29.151	29.120	42.414	1.00 25.51
HETATM	3627	O	HOH	1197	10.760	56.327	24.871	1.00 25.61
HETATM	3628	O	HOH	1198	19.161	31.540	33.429	1.00 41.50
HETATM	3629	O	HOH	1201	31.584	19.545	39.778	1.00 41.14
HETATM	3630	O	HOH	1202	31.499	33.130	31.243	1.00 30.94
HETATM	3631	O	HOH	1203	33.475	31.251	32.729	1.00 30.16
HETATM	3632	O	HOH	1204	25.323	26.251	24.066	1.00 29.38
HETATM	3633	O	HOH	1205	18.912	50.780	14.345	1.00 28.88
HETATM	3634	O	HOH	1206	28.562	46.055	22.818	1.00 37.71
HETATM	3635	O	HOH	1207	31.212	15.396	37.505	1.00 38.29
HETATM	3636	O	HOH	1208	21.188	13.368	44.376	1.00 22.37
HETATM	3637	O	HOH	1209	17.682	38.715	10.160	1.00 31.02
HETATM	3638	O	HOH	1210	50.214	11.867	37.111	1.00 50.09
HETATM	3639	O	HOH	1212	28.768	41.646	47.276	1.00 22.25
HETATM	3640	O	HOH	1214	49.993	18.233	34.806	1.00 44.55
HETATM	3641	O	HOH	1215	32.815	34.522	46.504	1.00 35.13
HETATM	3642	O	HOH	1216	39.893	28.328	41.896	1.00 12.01
HETATM	3643	O	HOH	1217	15.338	26.949	28.916	1.00 11.70
HETATM	3644	O	HOH	1218	35.548	32.617	33.681	1.00 18.33
HETATM	3645	O	HOH	1219	39.368	28.656	34.414	1.00 16.49
HETATM	3646	O	HOH	1220	10.631	22.205	16.485	1.00 23.48
HETATM	3647	O	HOH	1221	38.404	33.931	29.548	1.00 20.31
HETATM	3648	O	HOH	1222	29.170	43.940	45.652	1.00 17.85
HETATM	3649	O	HOH	1223	16.493	28.977	30.383	1.00 19.55
HETATM	3650	O	HOH	1224	50.201	26.750	43.278	1.00 23.76
HETATM	3651	O	HOH	1225	38.642	25.017	49.298	1.00 24.48
HETATM	3652	O	HOH	1226	22.132	37.260	38.648	1.00 21.90
HETATM	3653	O	HOH	1227	39.985	27.256	49.971	1.00 19.31
HETATM	3654	O	HOH	1228	46.680	26.589	41.727	1.00 24.34
HETATM	3655	O	HOH	1229	45.783	30.693	47.582	1.00 25.33
HETATM	3656	O	HOH	1230	37.132	23.521	50.764	1.00 25.39
HETATM	3657	O	HOH	1231	37.666	45.416	31.269	1.00 22.37
HETATM	3658	O	HOH	1232	12.017	34.217	29.751	1.00 24.35
HETATM	3659	O	HOH	1233	26.995	45.967	27.617	1.00 23.52
HETATM	3660	O	HOH	1234	26.536	25.536	28.250	1.00 29.21
HETATM	3661	O	HOH	1235	25.412	37.399	29.161	1.00 27.51
HETATM	3662	O	HOH	1236	37.339	31.390	35.413	1.00 25.38
HETATM	3663	O	HOH	1237	49.870	32.179	49.678	1.00 25.92
HETATM	3664	O	HOH	1238	22.061	39.616	17.387	1.00 15.04
HETATM	3665	O	HOH	1239	14.228	24.366	29.787	1.00 22.47
HETATM	3666	O	HOH	1240	23.022	47.566	29.327	1.00 39.50
HETATM	3667	O	HOH	1241	21.098	32.679	17.559	1.00 35.09
HETATM	3668	O	HOH	1242	23.864	37.449	16.707	1.00 37.28

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FIGURE 8A-72

HETATM	3669	O	HOH	1243	32.934	17.639	38.491	1.00 30.00
HETATM	3670	O	HOH	1244	30.081	39.275	47.475	1.00 27.25
HETATM	3671	O	HOH	1245	40.219	10.507	54.210	1.00 42.36
HETATM	3672	O	HOH	1246	20.198	57.839	14.584	1.00 26.12
HETATM	3673	O	HOH	1247	22.701	31.034	19.118	1.00 26.32
HETATM	3674	O	HOH	1248	50.529	25.000	51.117	1.00 16.36
HETATM	3675	O	HOH	1249	27.308	27.122	38.575	1.00 29.98
HETATM	3676	O	HOH	1250	41.664	46.630	31.018	1.00 29.42
HETATM	3677	O	HOH	1251	27.841	34.202	44.699	1.00 37.98
HETATM	3678	O	HOH	1252	28.946	26.204	44.341	1.00 51.94
HETATM	3679	O	HOH	1253	26.643	43.795	23.560	1.00 23.03
HETATM	3680	O	HOH	1254	52.894	25.886	44.095	1.00 33.52
HETATM	3681	O	HOH	1255	42.339	26.613	55.952	1.00 36.97
HETATM	3682	O	HOH	1256	48.804	2.432	50.876	1.00 36.59
HETATM	3683	O	HOH	1257	51.244	18.531	40.805	1.00 33.51
HETATM	3684	O	HOH	1260	49.903	39.828	48.137	1.00 44.77
HETATM	3685	O	HOH	1261	45.720	4.638	32.384	1.00 54.41
HETATM	3686	O	HOH	1262	32.871	29.567	30.088	1.00 39.72
HETATM	3687	O	HOH	1263	23.890	51.918	23.175	1.00 37.61
HETATM	3688	O	HOH	1264	13.550	26.049	31.905	1.00 33.45
HETATM	3689	O	HOH	1266	10.689	31.547	31.432	1.00 47.94
HETATM	3690	O	HOH	1269	26.086	-7.425	31.507	1.00 39.58
HETATM	3691	O	HOH	1271	22.022	54.673	22.853	1.00 37.03
HETATM	3692	O	HOH	1274	28.901	24.308	41.027	1.00 41.39
HETATM	3693	O	HOH	1276	45.609	-2.697	31.603	1.00 49.62
HETATM	3694	O	HOH	1277	9.649	26.708	34.475	1.00 36.02
HETATM	3695	O	HOH	1279	21.970	8.818	36.303	1.00 45.69
HETATM	3696	O	HOH	1280	7.956	56.039	27.031	1.00 55.41
HETATM	3697	O	HOH	1281	15.342	17.025	12.461	1.00 55.13
HETATM	3698	O	HOH	1284	12.862	44.437	3.810	1.00 49.95
HETATM	3699	O	HOH	1286	34.675	64.010	47.159	1.00 47.97
HETATM	3700	O	HOH	1287	41.049	11.857	30.681	1.00 29.94
HETATM	3701	O	HOH	1288	34.457	19.302	55.855	1.00 47.88
HETATM	3702	O	HOH	1289	28.546	31.433	28.564	1.00 47.71
HETATM	3703	O	HOH	1291	33.220	60.645	39.548	1.00 52.03
HETATM	3704	O	HOH	1292	30.910	54.312	27.471	1.00 48.06
HETATM	3705	O	HOH	1293	23.058	27.656	32.358	1.00 45.02
HETATM	3706	O	HOH	1294	28.377	27.865	25.772	1.00 37.73
HETATM	3707	O	HOH	1295	17.851	13.033	47.051	1.00 31.43
HETATM	3708	O	HOH	1297	22.435	24.151	33.420	1.00 39.38
HETATM	3709	O	HOH	1298	29.292	20.833	37.423	1.00 52.78
HETATM	3710	O	HOH	1299	26.196	40.554	47.655	1.00 52.83
HETATM	3711	O	HOH	1300	6.687	28.384	34.247	1.00 45.71
HETATM	3712	O	HOH	1303	41.624	1.272	27.661	1.00 61.55
HETATM	3713	O	HOH	1306	24.865	48.368	49.108	1.00 53.05
HETATM	3714	O	HOH	1308	43.375	33.196	54.115	1.00 34.68
HETATM	3715	O	HOH	1309	24.941	16.106	28.105	1.00 27.22
HETATM	3716	O	HOH	1310	48.767	36.362	53.067	1.00 39.18
HETATM	3717	O	HOH	1311	0.897	25.934	24.841	1.00 47.80
HETATM	3718	O	HOH	1312	41.531	54.883	30.082	1.00 37.92
HETATM	3719	O	HOH	1315	32.370	19.055	31.177	1.00 43.71
HETATM	3720	O	HOH	1316	19.469	15.072	45.662	1.00 48.16
HETATM	3721	O	HOH	1321	10.144	48.734	5.731	1.00 39.11
HETATM	3722	O	HOH	1322	29.076	56.977	42.203	1.00 46.38
HETATM	3723	O	HOH	1326	42.727	8.091	54.610	1.00 56.42
HETATM	3724	O	HOH	1330	41.316	20.071	29.052	1.00 39.86
HETATM	3725	O	HOH	1331	16.596	27.837	34.825	1.00 50.15
HETATM	3726	O	HOH	1332	19.903	45.162	47.256	1.00 52.33
HETATM	3727	O	HOH	1333	40.238	-8.133	39.062	1.00 41.11
HETATM	3728	O	HOH	1335	32.007	37.168	46.170	1.00 43.84

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FIGURE 8A-73

HETATM 3729	O	HOH	1337	8.866	32.982	29.638	1.00	51.57
HETATM 3730	O	HOH	1339	35.650	46.023	29.211	1.00	40.99
HETATM 3731	O	HOH	1340	52.825	32.335	38.756	1.00	50.57
HETATM 3732	O	HOH	1341	36.938	51.807	31.314	1.00	45.30
HETATM 3733	O	HOH	1342	18.790	42.705	33.580	1.00	43.47
HETATM 3734	O	HOH	1344	22.819	36.661	11.619	1.00	46.70
HETATM 3735	O	HOH	1345	19.465	28.669	34.714	1.00	39.89
HETATM 3736	O	HOH	1347	40.179	23.790	53.530	1.00	47.43
HETATM 3737	O	HOH	1353	3.487	36.484	13.806	1.00	40.41
HETATM 3738	O	HOH	1360	31.223	4.884	34.089	1.00	30.96
HETATM 3739	O	HOH	1361	19.647	3.819	14.444	1.00	26.16
HETATM 3740	O	HOH	1364	12.171	-3.712	34.829	1.00	52.07
HETATM 3741	O	HOH	1366	14.715	10.503	15.414	1.00	47.98
HETATM 3742	O	HOH	1370	3.284	18.073	30.684	1.00	39.22
HETATM 3743	O	HOH	1371	16.114	12.267	13.222	1.00	41.79
HETATM 3744	O	HOH	1374	26.710	-10.158	28.570	1.00	46.72
HETATM 3745	O	HOH	1376	13.842	2.095	17.391	1.00	51.23
HETATM 3746	O	HOH	1377	23.624	18.176	26.993	1.00	46.55
HETATM 3747	O	HOH	1378	17.679	9.897	14.906	1.00	29.42
HETATM 3748	O	HOH	1380	21.173	-2.881	15.825	1.00	44.25
HETATM 3749	O	HOH	1381	25.990	6.184	14.411	1.00	40.98
HETATM 3750	O	HOH	1382	25.475	8.938	15.031	1.00	40.93
HETATM 3751	O	HOH	1384	27.045	17.549	12.911	1.00	44.46
HETATM 3752	O	HOH	1387	15.174	-5.506	13.111	1.00	43.09
HETATM 3753	O	HOH	1388	3.093	25.580	28.841	1.00	47.33
HETATM 3754	O	HOH	1389	43.833	14.822	32.665	1.00	30.09
HETATM 3755	O	HOH	1390	27.283	3.257	16.277	1.00	28.50
HETATM 3756	O	HOH	1391	31.590	8.583	17.790	1.00	31.43
HETATM 3757	O	HOH	1392	28.183	8.699	15.618	1.00	37.69
HETATM 3758	O	HOH	1393	24.599	3.854	15.072	1.00	40.30
HETATM 3759	O	HOH	1404	39.148	30.436	32.035	1.00	17.64
HETATM 3760	O	HOH	1405	0.837	22.245	22.324	1.00	55.83
HETATM 3761	O	HOH	1406	29.799	34.134	27.910	1.00	28.75
HETATM 3762	O	HOH	1407	18.445	6.222	44.059	1.00	53.71
HETATM 3763	O	HOH	1409	30.392	39.323	25.039	1.00	34.89
HETATM 3764	O	HOH	1410	18.490	9.793	47.086	1.00	48.51
HETATM 3765	O	HOH	1411	13.220	32.748	8.629	1.00	49.26
HETATM 3766	O	HOH	1412	49.361	20.100	32.438	1.00	43.65
HETATM 3767	O	HOH	1414	51.855	33.864	41.242	1.00	64.26
HETATM 3768	O	HOH	1418	47.727	41.100	41.717	1.00	35.47
HETATM 3769	O	HOH	1419	24.466	54.548	43.747	1.00	53.28
HETATM 3770	O	HOH	1420	5.934	30.983	8.318	1.00	45.39
HETATM 3771	O	HOH	1421	32.399	-4.433	42.259	1.00	41.31
HETATM 3772	O	HOH	1422	3.024	40.996	27.927	1.00	42.40
HETATM 3773	O	HOH	1424	36.321	-0.489	35.913	1.00	41.12
HETATM 3774	O	HOH	1428	16.200	42.165	4.789	1.00	62.98
HETATM 3775	O	HOH	1429	4.930	40.213	24.269	1.00	53.41
HETATM 3776	O	HOH	1430	7.506	9.248	13.243	1.00	51.74
HETATM 3777	O	HOH	1434	16.093	51.978	11.936	1.00	39.24
HETATM 3778	O	HOH	1437	32.063	21.866	31.547	1.00	49.87
HETATM 3779	O	HOH	1438	54.621	26.247	29.147	1.00	48.62
HETATM 3780	O	HOH	1440	4.318	19.369	8.919	1.00	47.53
HETATM 3781	O	HOH	1441	5.136	2.358	29.831	1.00	44.25
HETATM 3782	O	HOH	1443	2.076	24.174	15.211	1.00	53.91
HETATM 3783	O	HOH	1444	15.474	42.729	30.690	1.00	38.63
HETATM 3784	O	HOH	1446	34.955	9.442	53.656	1.00	51.40
HETATM 3785	O	HOH	1447	28.597	17.387	31.041	1.00	40.53
HETATM 3786	O	HOH	1454	34.884	-9.534	12.912	1.00	33.84
HETATM 3787	O	HOH	1455	56.971	31.610	49.136	1.00	44.36
HETATM 3788	O	HOH	1456	29.676	11.548	53.175	1.00	41.64

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FIGURE 8A-74

```
HETATM 3789   O   HOH  1457     46.713  47.217  35.996  1.00 51.75        O
HETATM 3790   O   HOH  1458     22.556   3.172  12.871  1.00 35.99        O
HETATM 3791   O   HOH  1459     42.572  42.347  52.583  1.00 55.24        O
HETATM 3792   O   HOH  1461      0.573  13.064. 16.484  1.00 44.57        O
HETATM 3793   O   HOH  1462     50.467   6.260  32.228  1.00 46.40        O
HETATM 3794   O   HOH  1463      6.167  47.337   5.349  1.00 53.27        O
HETATM 3795   O   HOH  1464     24.604  -9.866  26.249  1.00 43.72        O
HETATM 3796   O   HOH  1466     22.806  17.220  45.236  1.00 61.41        O
HETATM 3797   O   HOH  1506     25.441  49.608  19.993  1.00 33.89        O
HETATM 3798   O   HOH  1507     39.709  -9.399  16.482  1.00 30.44        O
HETATM 3799   O   HOH  1509      9.926  24.411  36.529  1.00 37.21        O
HETATM 3800   O   HOH  1515     34.731  28.232  28.355  1.00 37.81        O
HETATM 3801   O   HOH  1518     44.323  37.583  28.523  1.00 44.08        O
HETATM 3802   O   HOH  1519     30.194  -0.768  45.229  1.00 40.11        O
HETATM 3803   O   HOH  1521     42.425  48.375  34.242  1.00 50.42        O
HETATM 3804   O   HOH  1523     12.185   2.224  34.335  1.00 56.22        O
CONECT   109  108  110  119
CONECT   119  109  120
CONECT   120  119  121  123
CONECT   121  120  122  127
CONECT   122  121
CONECT   123  120  124
CONECT   124  123  125
CONECT   125  124  126
CONECT   126  125
CONECT   127  121  128
CONECT   187  186  188  189
CONECT   189  187  190
CONECT   190  189  191  193
CONECT   191  190  192  197
CONECT   192  191
CONECT   193  190  194
CONECT   194  193  195
CONECT   195  194  196
CONECT   196  195
CONECT   197  191  198
CONECT   248  247  905
CONECT   279  278  280  286
CONECT   286  279  287
CONECT   287  286  288  290
CONECT   288  287  289  294
CONECT   289  288
CONECT   290  287  291
CONECT   291  290  292
CONECT   292  291  293
CONECT   293  292
CONECT   294  288  295
CONECT   905  248  904
CONECT  1038 1037 1039 1048
CONECT  1048 1038 1049
CONECT  1049 1048 1050 1052
CONECT  1050 1049 1051 1056
CONECT  1051 1050
CONECT  1052 1049 1053
CONECT  1053 1052 1054
CONECT  1054 1053 1055
CONECT  1055 1054
CONECT  1056 1050 1057
CONECT  1116 1115 1117 1118
CONECT  1118 1116 1119
```

Applicants: *Wayne A. Hendrickson , et al.*
U.S. Serial No: 09/609,207
Filing Date: June 29, 2000
Title of the Invention: Conjugated Ligands
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FIGURE 8A-75

```
CONECT 1119 1118 1120 1122
CONECT 1120 1119 1121 1126
CONECT 1121 1120
CONECT 1122 1119 1123
CONECT 1123 1122 1124
CONECT 1124 1123 1125
CONECT 1125 1124
CONECT 1126 1120 1127
CONECT 1177 1176 1874
CONECT 1208 1207 1209 1215
CONECT 1215 1208 1216
CONECT 1216 1215 1217 1219
CONECT 1217 1216 1218 1223
CONECT 1218 1217
CONECT 1219 1216 1220
CONECT 1220 1219 1221
CONECT 1221 1220 1222
CONECT 1222 1221
CONECT 1223 1217 1224
CONECT 1874 1177 1873
CONECT 1987 1986 1988 1997
CONECT 1997 1987 1998
CONECT 1998 1997 1999 2001
CONECT 1999 1998 2000 2005
CONECT 2000 1999
CONECT 2001 1998 2002
CONECT 2002 2001 2003
CONECT 2003 2002 2004
CONECT 2004 2003
CONECT 2005 1999 2006
CONECT 2065 2064 2066 2067
CONECT 2067 2065 2068
CONECT 2068 2067 2069 2071
CONECT 2069 2068 2070 2075
CONECT 2070 2069
CONECT 2071 2068 2072
CONECT 2072 2071 2073
CONECT 2073 2072 2074
CONECT 2074 2073
CONECT 2075 2069 2076
CONECT 2154 2153 2155 2161
CONECT 2161 2154 2162
CONECT 2162 2161 2163 2165
CONECT 2163 2162 2164 2169
CONECT 2164 2163
CONECT 2165 2162 2166
CONECT 2166 2165 2167
CONECT 2167 2166 2168
CONECT 2168 2167
CONECT 2169 2163 2170
CONECT 2813 2812 2814 2823
CONECT 2823 2813 2824
CONECT 2824 2823 2825 2827
CONECT 2825 2824 2826 2831
CONECT 2826 2825
CONECT 2827 2824 2828
CONECT 2828 2827 2829
CONECT 2829 2828 2830
CONECT 2830 2829
CONECT 2831 2825 2832
```

Applicants: Wayne A. Hendrickson, et al.
U.S. Serial No: 09/609,207
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FIGURE 8A-76

```
CONECT 2891 2890 2892 2893
CONECT 2893 2891 2894
CONECT 2894 2893 2895 2897
CONECT 2895 2894 2896 2901
CONECT 2896 2895
CONECT 2897 2894 2898
CONECT 2898 2897 2899
CONECT 2899 2898 2900
CONECT 2900 2899
CONECT 2901 2895 2902
CONECT 2983 2982 2984 2990
CONECT 2990 2983 2991
CONECT 2991 2990 2992 2994
CONECT 2992 2991 2993 2998
CONECT 2993 2992
CONECT 2994 2991 2995
CONECT 2995 2994 2996
CONECT 2996 2995 2997
CONECT 2997 2996
CONECT 2998 2992 2999
CONECT 3522 3541 3542
CONECT 3524 3544 3545 3546
CONECT 3525 3526
CONECT 3526 3525 3527
CONECT 3527 3526 3528
CONECT 3528 3527 3530
CONECT 3529 3530 3531
CONECT 3530 3528 3529
CONECT 3531 3529 3533
CONECT 3532 3533 3534
CONECT 3533 3531 3532
CONECT 3534 3532 3536
CONECT 3535 3536 3537
CONECT 3536 3534 3535
CONECT 3537 3535 3539
CONECT 3538 3539 3540
CONECT 3539 3537 3538
CONECT 3540 3538
CONECT 3541 3522
CONECT 3542 3522
CONECT 3544 3524
CONECT 3545 3524
CONECT 3546 3524
MASTER        301    0   16   19    8    0    0   27 3796    4  147   84
END
```